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Denovo Structural Modeling and B cell and T cell Epitope Prediction against SARS-COV-2 PLpro to Cure COVID-19: Vaccinomics Based Approach

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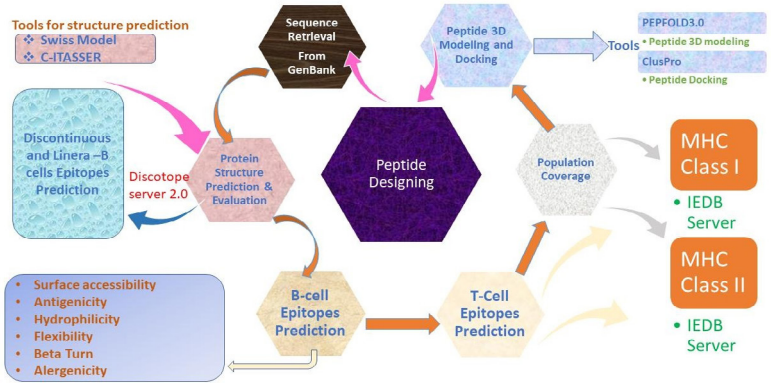
Abstract

Background: In December 2019, SARS COV-2 spread very rapidly and its outbreaks led to cause pneumonia and severe illness. For the first time, the virus was spotted in the city of China (Wuhan). Little is known about this virus, so the vaccine is needed to prevent COVID-19. Papain like protease (PLpro) is conserved among coronaviruses and have multifunctional activities like protease, deubiquitinase, deISGylating and interferon antagonism. Therefore, PLpro is a promising target for drug and vaccine development.

Methods: T cells (MHCI & MHCII) and B cell (Discontinuous & Linear) epitopes of SARS COV-2 PLpro were forecasted via computational and immunoinformatics approaches that show a crucial part in promoting immune responses against COVID-19. Online tools were used to analyze the allergenicity, physiochemical properties, antigenicity and structural details of PLpro.

Results: Fifty-three Linear B-cell epitopes were identified, of which 'KPLEFGATSAALQP' and 'EDDYQGKPLEFGAT' had higher score and antigenicity. Antigenic, non-allergenic and conserved (T cell) epitopes whichwere bounded to multiple alleles were selected. In total, twelve epitopes were taken (6 MHC I and 6 MHC II).From MHC class I 'YHTTDPSFLGRY' and MHC class II 'PFVMMSAPPAQYELK' had more antigenicity among T cell epitopes. Furthermore, the protection and stability of peptides were tested through digestion analysis.

Conclusion: Predicted epitopes could be served as vaccine candidate to eliminate COVID-19. Even so, the presented epitopes required to be validated experimentally to check its safety and immunogenic profile



Graphical Abstract

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Keywords: Papain like protease; Digestion analysis; Allergenicity; Antigenicity

Introduction

Coronaviruses are positive-sense RNA viruses which are widely spread among humans and many other species of mammals [1]. Two types of coronaviruses such as SARS-CoV [2-4] and MERS-CoV [5, 6] cause infection and more than 10,000 cases have been reported in the past two decades. In December 2019, numerous incidences of an unknown cause of COVID-19 occurred in Wuhan, Hubei, China, with the clinical presentations closely similar to viral pneumonia [7]. The cause of the cases of pneumonia was reported as a novel beta coronavirus, SARS-CoV- 2.The genome of SARS-CoV-2 includes 3-chymotrypsin like protease (3CLpro), papain-like protease (PLpro), RNA-dependant-RNA polymerase andstructural proteins (spike glycoprotein, Envelope, membrane and nucleoprotein).Sequence analysis of SARS-CoV-2 revealed, receptor- binding domain(RBD) and receptor binding motif(RBM) together interact with the receptor angiotensin enzyme 2(ACE2)[8, 9].

SARS-CoV-2identified through deep sequence analysis and more than 800 cases reported in Wuhan and various cases reported in Japan, Thailand, South Korea and the USA. This novel coronavirus was discovered by NHC Key Laboratory of System Biology and Christophe Meraux, China that was confirmed by the WHO[10].WHO declared the public health risks about coronavirus in January 2020 and also gave information that there is no vaccine approved till now[9]. It is confirmed through phylogenetic analysis that the origin of Coronavirus is a bat that transmitted human to human by droplets/air. Infected persons have symptoms such as diarrhea, thrombocytopenia, fever, and respiratory disorders. Further analysis has been made by Real Time-PCR for the gene coding internal RNA-RNA dependent polymerase and Spike's receptor- binding domain and these analyses after that conformed through Sanger Sequencing and full genome analysis is done by Next Generation Sequencing(NGS)[11-13].The mentioned nonstructural proteins such as PLpro, RNA-RNA dependent polymerase and chymotrypsin-like protease are conserved among all types of coronaviruses, therefore, these proteins could be used as strong antiviral targets to develop a vaccine against SARS and MERS[13].

At present time, no vaccine is availableto cure coronavirus infection in humans. Traditionally two medicines such as ShuFengJieDu and Lianhuaqingwen capsules are usedto treat COVID-19 in China [14]. Many other options could be used for the treatment of SARS-CoV-2 such as vaccines, peptides, monoclonal-oligonucleotides based therapies, and small molecule drugs but these preventive methods need months to years for the development [15].

The purpose of immunization is to design vaccines that have to initiate rapid immune response against pathogen's antigen. In Vitro vaccine designing could be expensive,time exhausting and there is a need to culture the viruses which is not safe biologically[16]. In immunoinformatic,there is no need to culture viruses and it is biologically safe.B-cells and T- cells are important cells of the immune system that produce immune responses. Immunoinformatics is sub-field of bioinformatics that consist of many bioinformatics tools and databases. Immunological data prediction have been done with the help of these tools. In the advancement of tools, now it has been easy for the scientists to predict B-cell and T-cell epitopes [17] for the development of vaccine sub-unit construct [18, 19]. The basic mechanism to design the peptide vaccine is the prediction of the B-celland T-cell epitopes that are antigenic having particular immune-responses [20]. Therapeutic strategies for the treatment of the E-bola, Zika, and MERS-COV viruses have been designed by the use ofthe in silico peptide prediction approach in various studies [21-23]. The recent study was designed to predict epitopes from SARS-COV-2 PLpro which may be helpful to develop vaccine in future.

Methodology

Protein structure analysis/Physiochemical Properties prediction of PLpro

The protein sequence of PLpro was taken from Genbank(ID: QHD43415.1)[24]. To evaluate the chemical and physical properties of PLpro the Expasy ProtParam tool was used [25]. GOR4 was used to analyze the protein's secondary structure. Protein's transmembrane topology was analyzed usingthe TMHMM tool. Di-sulphide-bonds of the protein were forecasted by DIANNA v1.1[26]. Antigenicity and Allergenicity of protein werepredicted viaVAXIJEN & ALLERTOP servers [27, 28].

3D Structure Prediction & Validation

The tertiary structure of the PLpro was identified through different online tools like Phyre 2,Swissmodel, C-I tasser and Raptor x[29-31]. Galaxy refine server was used to refine the retrieved model [32]. The refined structure was then checked in PROSA web server that offers a quality factor. The quality-factor suggests a potential protein structure defect, beyond the usual range of native proteins [33]. Ramachandran plot was created with the PROCHECK principle via rampage server to validate the refined structure [34]. To evaluate the details of unbounded interactions, ERRAT server was used [35].

Prediction of B-cell epitopes

B-cell epitopes help in defending the immune-system. ABC-PRED was applied to identify B- cell epitopes with the threshold value of 0.51[36]. Epitopes visible on the surface were selected for antigenicity testing via VaxiJen server at 0.5 threshold. Kolaskar and Tongaonkar Antigenicity scale, Parkar hydrophilicity prediction algorithm, Karplus and Schulz flexibility prediction tool, Emini surface accessibility

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prediction method were applied to execute antigenicity, hydrophilicity, flexibility, surface accessibility analysis respectively [37]. As discontinuous epitopes have higher dominant properties than linear epitopes and are more evident. Discontinuous epitopes were identified through DiscoTope 2.0server using three- dimensional structure of PLpro protein [38]. Pymol was applied to visualize the location of epitopes on the 3D protein structure [39].

T-cell epitopes prediction

T-cell epitopes have avital role in designing of a vaccine. MHC-I &MHCII T cell epitopes were predicted through the IEDB database having a length of peptides 12 and 15 mer respectively[40].HLA alleles were chosen in large numbers so that epitope prediction should be accurate. For prediction, all the alleles were selected and the sequence was given in FASTA format. T-cell epitopes having lower ranking score which is less than 2.0 considered good binders and could be used for further research.

Conservation Analysis of Epitopes

Conservation analysis was done by the IEDB server database. Epitopes with 100% conservation were selected[41].

Population Coverage Estimation

The distribution and expression of HLA alleles dependupon the world's regions and ethnicities, therefore impacting the efficient production of an epitope-based vaccine [42]. In this study selected MHC class I and MHC class II epitopes and related HLA alleles were used for population coverage analisis via IEDB population coverage tool [43]. Population coverage of each epitope was estimated in the regions where SARS-COV-2 cases were reported.

Properties Evaluation of Peptides

Expassy Protparam tool was applied to check the physiochemical properties of peptides like molecular weight and theoretical pI. VaxiJen v 2.0 and Allergen Fp 1.0 was used to forecast Antigenicity and Allergenicity of the peptide [44]. Toxic and non-toxic peptide prediction was done by ToxinPred but for further analysis, non-toxic peptide was selected [45]. To forecast peptide digester enzymes; the protein-digesting enzyme server was used.

Peptides Modeling and Docking

PEPFOLD was applied for the prediction of tertiary structures of six MHC I epitopes. PEPFOLD creates five models for each peptide and the best model was picked for further work [46]. 3D structure of the HLA –B7 allele was downloaded from PDB (ID: 3VCL).ClusPro (v.2) was used for molecular docking [47].

Results

Sequence retrieval & structural analysis

ProtParam was used to evaluate physiochemical properties of SARS COV-2 PLpro. Protein is in stable form, acidic and hydrophilic and has molecular weight 217252.61 kDa. Antigenicity and allergenicity of this sequence weretested by AllerTop and VaxiJen respectively. The results indicate thenon-allergenic and antigenic nature of proteinhaving an antigenicity value of0.5142. DIANNA v1.1 was used to evaluate 51 disulphide bonds of protein (Additional file 1: Table S1). Four transmembrane helices were predicted through TMHMM. Residues of protein that were on transmembrane helix were from 1413-1435, 1500-1522, 1532-1554 and 1561-1583. Residues from 1-1412, 1523-1531 and 1584-1945 were found on the outer surface. Protein residues from 1436-1499 and 1555-1560 were found in the inner surface of the core region. GOR4was used to forecast the details of the secondary structure of the target protein. Among the 1945 amino acids, the formation of α-helix consists of 508 amino acids representing 26.12%, 472 in beta strands representing 24.27% and 965 amino acids forms coils representing 49.61% of the total protein composition.

Tertiary Structure Prediction and Validation

Models retrieved from the Swiss model, C-I Tasser, Raptor x and Phyre 2 were evaluated by Ramachandran plot analysis.The model retrieved from the Swiss Model was best compared to other resources.The protein homology model based on the quality of QMEAN was developed in the Swiss Model. It providesQMean value and GMQE(Global Model Quality Estimation) value.GMQE represents the certainty of a model considering the coverage, arrangement of the target and the template.Higher GMQE value represents a better quality of the model. It is usually measuredin the range of 0 and 1.GMQE of the model was 0.11 and QMean was -0.28 which indicates the high quality of the protein structure. The best template was found to be 3e9s having a sequence identity of 82.86%(Figure 1a).The model was then refined by the Galaxy refine server.The improved model has 98.1% favored region in RAMPAGE and poor rotamers as 0.4%, qrmsd as 0.298, clash score as 10.6, MolProbity as 1.542(Figure 1c). ProSA-web also gives−9.02 Z, which is within an acceptable range (Figure 1b). These results show that the refined model has goodquality.

B cell epitopes prediction

B cell epitope of target protein was checked by ABCpred and TMHMM server were used to check surface availabity. VaxiJen was used to find the antigenicity of the epitopes. Epitopes that were 100% conserved, evident on the surface and antigenic were picked. A Total of 53 epitopes was chosen. 'KPLEFGATSAALQP' and 'EDDYQGKPLEFGAT' had high Antigenicity (1.7) and score(Table 1). We used Pymol to visualize the position of epitopes on the protein(Figure 2). Besides, surface accessibility of B cell epitopes was assessed. Through observing their concentration in previously identified B cell epitopes and physiochemical properties, the

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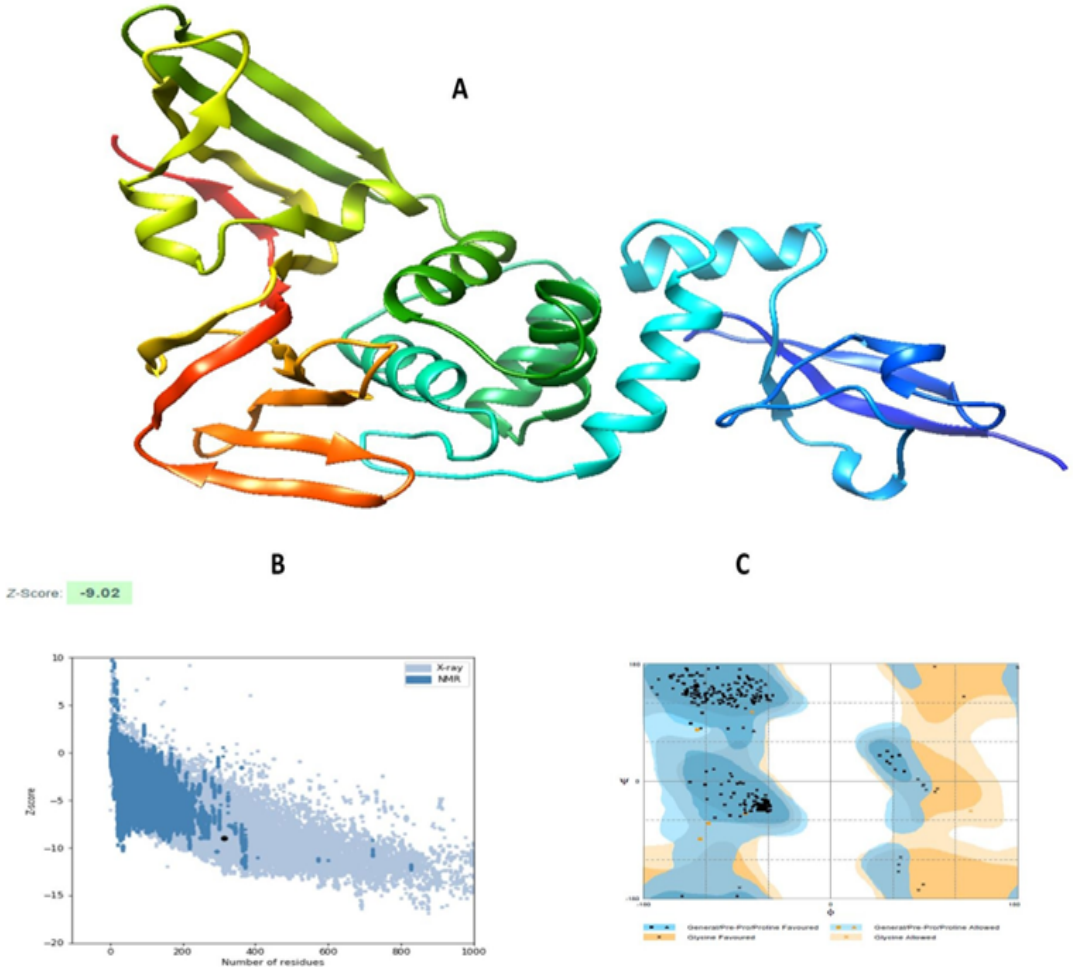

Figure 1: (a) 3D structural representation of PLpro protein predicted by Swiss Model (b) the z- score (-9.02) of the PLproprotein; (c) the Ramachandran plot of refined structure shows 98.1, 1.9% and 0.0% residues in favored, allowed and disallowed region, respectively.

target protein was evaluatedfor prediction of B cell epitopes by Kolaskar and Tongaonkar antigenicity tool.Window size and a threshold werekept at 7 and 1.045 respectively. The antigenic propensity value of PLpro was predicted as 1.041 Average, 0.859 Minimum and 1.258 Maximum(Figure 3A). Experimental research reveals that antibodies or alleles binding section of epitopes is elastic. Hydrophilic protein areas have a role in triggering an immune response and usually have surface exposure.Vaxijen antigenic value and the ABCpred score indicate that all predicted epitopes belong to the extracellular area of transmembrane proteins, which might boost a host defensive reaction during SARS-COV-2 infection. The parker hydrophilicity prediction algorithm with a threshold of 1.279 was used to evaluate hydrophilicity.Values calculated by parker hydrophilicity were 1.409Average, -8.971 Minimum and 8.129 Maximum(Figure 3C). Emini surface accessibility prediction method with a threshold of 1.009 was used to calculate the surface abundance of potential B cell epitopes. Additional file 2 (Table S2)contains the findings of the Emini surface accessibility(Figure 3D). Chou and Fasman beta-turn analyzing algorithm was used for the prediction of beta-turn because beta-turns play a vital role in initiating the defensive response. Beta-turns are hydrophilic and exposed to the surface. It calculated the values of 0.973Average, 0.593Minimum and 1.414 Maximum at the threshold of 1.009. The results show that the area from 1098-1104 amino acids and 1849-1855 amino acids are more likely to persuade beta turns in peptide structure(Figure 3B).Flexibility analysis by Karplus and schulz tool showed that the area from673-679 amino acids is highly versatile (Figure 3E).

DiscoTope 2.0 server was applied to trackthe surface abundance of residual contact numbers and use the novel amino acid score to preview discontinuous epitopes to further improve the specificity and variety of B cell epitopes.At − 3.700 threshold, 22.000 Angstroms propensity score radius and 90% specificity, twenty-nine discontinuous epitopes were identified from the 3D structure of the protein (Table 2). Pymol visualized the location of epitopes on the 3D protein structure (Figure 4).

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Table 1: Emini Surface accessibility of PLpro predicted by EMINI surface accessibility tool

Position	Residue	Start	End	Peptide	Score
3	**T**	1	6	APTKVT	1.1
4	**K**	2	7	PTKVTF	0.943
5	**V**	3	8	TKVTFG	0.604
6	**T**	4	9	KVTFGD	0.698
7	**F**	5	10	VTFGDD	0.583
8	**G**	6	11	TFGDDT	1.134
9	**D**	7	12	FGDDTV	0.583
10	**D**	8	13	GDDTVI	0.472
11	**T**	9	14	DDTVIE	0.826
12	**V**	10	15	DTVIEV	0.367
13	**I**	11	16	TVIEVQ	0.381
14	**E**	12	17	VIEVQG	0.261
15	**V**	13	18	IEVQGY	0.551
16	**Q**	14	19	EVQGYK	1.573
17	**G**	15	20	VQGYKS	1.217
18	**Y**	16	21	QGYKSV	1.217
19	**K**	17	22	GYKSVN	1.13
20	**S**	18	23	YKSVNI	0.8
21	**V**	19	24	KSVNIT	0.737
22	**N**	20	25	SVNITF	0.319
23	**I**	21	26	VNITFE	0.413
24	**T**	22	27	NITFEL	0.458
25	**F**	23	28	ITFELD	0.476
26	**E**	24	29	TFELDE	1.176
27	**L**	25	30	FELDER	1.596
28	**D**	26	31	ELDERI	1.292
29	**E**	27	32	LDERID	1.246
30	**R**	28	33	DERIDK	3.021
31	**I**	29	34	ERIDKV	1.343
32	**D**	30	35	RIDKVL	0.639
33	**K**	31	36	IDKVLN	0.525
34	**V**	32	37	DKVLNE	1.297
35	**L**	33	38	KVLNEK	1.553
36	**N**	34	39	VLNEKC	0.416
37	**E**	35	40	LNEKCS	0.752
38	**K**	36	41	NEKCSA	0.921
39	**C**	37	42	EKCSAY	0.897
40	**S**	38	43	KCSAYT	0.748
41	**A**	39	44	CSAYTV	0.278
42	**Y**	40	45	SAYTVE	0.897
43	**T**	41	46	AYTVEL	0.552
44	**V**	42	47	YTVELG	0.54
45	**E**	43	48	TVELGT	0.498
46	**L**	44	49	VELGTE	0.597
47	**G**	45	50	ELGTEV	0.597

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48	**T**	46	51	LGTEVN	0.555
49	**E**	47	52	GTEVNE	1.165
50	**V**	48	53	TEVNEF	1.019
51	**N**	49	54	EVNEFA	0.713
52	**E**	50	55	VNEFAC	0.221
53	**F**	51	56	NEFACV	0.221
54	**A**	52	57	EFACVV	0.102
55	**C**	53	58	FACVVA	0.059
56	**V**	54	59	ACVVAD	0.115
57	**V**	55	60	CVVADA	0.115
58	**A**	56	61	VVADAV	0.159
59	**D**	57	62	VADAVI	0.15
60	**A**	58	63	ADAVIK	0.404
61	**V**	59	64	DAVIKT	0.577
62	**I**	60	65	AVIKTL	0.285
63	**K**	61	66	VIKTLQ	0.489
64	**T**	62	67	IKTLQP	1.018
65	**L**	63	68	KTLQPV	1.078
66	**Q**	64	69	TLQPVS	0.722
67	**P**	65	70	LQPVSE	0.867
68	**V**	66	71	QPVSEL	0.867
69	**S**	67	72	PVSELL	0.413
70	**E**	68	73	VSELLT	0.385
71	**L**	69	74	SELLTP	0.803
72	**L**	70	75	ELLTPL	0.494
73	**T**	71	76	LLTPLG	0.282
74	**P**	72	77	LTPLGI	0.24
75	**L**	73	78	TPLGID	0.486
76	**G**	74	79	PLGIDL	0.278
77	**I**	75	80	LGIDLD	0.3
78	**D**	76	81	GIDLDE	0.63
79	**L**	77	82	IDLDEW	0.669
80	**D**	78	83	DLDEWS	1.279
81	**E**	79	84	LDEWSM	0.758
82	**W**	80	85	DEWSMA	0.928
83	**S**	81	86	EWSMAT	0.802
84	**M**	82	87	WSMATY	0.726
85	**A**	83	88	SMATYY	1.082
86	**T**	84	89	MATYYL	0.666
87	**Y**	85	90	ATYYLF	0.582
88	**Y**	86	91	TYYLFD	0.963
89	**L**	87	92	YYLFDE	1.155
90	**F**	88	93	YLFDES	0.988
91	**D**	89	94	LFDESG	0.624
92	**E**	90	95	FDESGE	1.31
93	**S**	91	96	DESGEF	1.31
94	**G**	92	97	ESGEFK	1.569

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95	**E**	93	98	SGEFKL	0.747
96	**F**	94	99	GEFKLA	0.563
97	**K**	95	100	EFKLAS	0.763
98	**L**	96	101	FKLASH	0.599
99	**A**	97	102	KLASHM	0.685
100	**S**	98	103	LASHMY	0.537
101	**H**	99	104	ASHMYC	0.349
102	**M**	100	105	SHMYCS	0.463
103	**Y**	101	106	HMYCSF	0.299
104	**C**	102	107	MYCSFY	0.344
105	**S**	103	108	YCSFYP	0.538
106	**F**	104	109	CSFYPP	0.531
107	**Y**	105	110	SFYPPD	1.654
108	**P**	106	111	FYPPDE	2.138
109	**P**	107	112	YPPDED	4.123
110	**D**	108	113	PPDEDE	4.557
111	**E**	109	114	PDEDEE	5.103
112	**D**	110	115	DEDEEE	5.716
113	**E**	111	116	EDEEEG	3.387
114	**E**	112	117	DEEEGD	3.266
115	**E**	113	118	EEEGDC	1.048
116	**G**	114	119	EEGDCE	1.048
117	**D**	115	120	EGDCEE	1.048
118	**C**	116	121	GDCEEE	1.048
119	**E**	117	122	DCEEEE	1.835
120	**E**	118	123	CEEEEF	0.951
121	**E**	119	124	EEEEFE	3.073
122	**E**	120	125	EEEFEP	2.744
123	**F**	121	126	EEFEPS	2.123
124	**E**	122	127	EFEPST	1.77
125	**P**	123	128	FEPSTQ	1.77
126	**S**	124	129	EPSTQY	3.202
127	**T**	125	130	PSTQYE	3.202
128	**Q**	126	131	STQYEY	3.245
129	**Y**	127	132	TQYEYG	2.396
130	**E**	128	133	QYEYGT	2.396
131	**Y**	129	134	YEYGTE	2.396
132	**G**	130	135	EYGTED	2.554
133	**T**	131	136	YGTEDD	2.463
134	**E**	132	137	GTEDDY	2.463
135	**D**	133	138	TEDDYQ	4.309
136	**D**	134	139	EDDYQG	2.955
137	**Y**	135	140	DDYQGK	3.412
138	**Q**	136	141	DYQGKP	3.16
139	**G**	137	142	YQGKPL	1.56
140	**K**	138	143	QGKPLE	1.725
141	**P**	139	144	GKPLEF	0.862

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142	**L**	140	145	KPLEFG	0.862
143	**E**	141	146	PLEFGA	0.436
144	**F**	142	147	LEFGAT	0.407
145	**G**	143	148	EFGATS	0.661
146	**A**	144	149	FGATSA	0.385
147	**T**	145	150	GATSAA	0.45
148	**S**	146	151	ATSAAL	0.375
149	**A**	147	152	TSAALQ	0.642
150	**A**	148	153	SAALQP	0.688
151	**L**	149	154	AALQPE	0.889
152	**Q**	150	155	ALQPEE	1.525
153	**P**	151	156	LQPEEE	2.613
154	**E**	152	157	QPEEEQ	5.488
155	**E**	153	158	PEEEQE	5.488
156	**E**	154	159	EEEQEE	6.147
157	**Q**	155	160	EEQEED	5.927
158	**E**	156	161	EQEEDW	3.599
159	**E**	157	162	QEEDWL	1.714
160	**D**	158	163	EEDWLD	1.653
161	**W**	159	164	EDWLDD	1.593
162	**L**	160	165	DWLDDD	1.537
163	**D**	161	166	WLDDDS	1.233
164	**D**	162	167	LDDDSQ	2.031
165	**D**	163	168	DDDSQQ	4.265
166	**S**	164	169	DDSQQT	3.686
167	**Q**	165	170	DSQQTV	1.638
168	**Q**	166	171	SQQTVG	0.971
169	**T**	167	172	QQTVGQ	1.254
170	**V**	168	173	QTVGQQ	1.254
171	**G**	169	174	TVGQQD	1.21
172	**Q**	170	175	VGQQDG	0.829
173	**Q**	171	176	GQQDGS	1.498
174	**D**	172	177	QQDGSE	2.621
175	**G**	173	178	QDGSED	2.527
176	**S**	174	179	DGSEDN	2.347
177	**E**	175	180	GSEDNQ	2.434
178	**D**	176	181	SEDNQT	3.549
179	**N**	177	182	EDNQTT	3.822
180	**Q**	178	183	DNQTTT	3.185
181	**T**	179	184	NQTTTI	1.337
182	**T**	180	185	QTTTIQ	1.44
183	**T**	181	186	TTTIQT	1.2
184	**I**	182	187	TTIQTI	0.583
185	**Q**	183	188	TIQTIV	0.3
186	**T**	184	189	IQTIVE	0.36
187	**I**	185	190	QTIVEV	0.381
188	**V**	186	191	TIVEVQ	0.381

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189	**E**	187	192	IVEVQP	0.408
190	**V**	188	193	VEVQPQ	1.008
191	**Q**	189	194	EVQPQL	1.12
192	**P**	190	195	VQPQLE	1.12
193	**Q**	191	196	QPQLEM	1.493
194	**L**	192	197	PQLEME	1.493
195	**E**	193	198	QLEMEL	0.796
196	**M**	194	199	LEMELT	0.664
197	**E**	195	200	EMELTP	1.245
198	**L**	196	201	MELTPV	0.533
199	**T**	197	202	ELTPVV	0.4
200	**P**	198	203	LTPVVQ	0.4
201	**V**	199	204	TPVVQT	0.7
202	**V**	200	205	PVVQTI	0.34
203	**Q**	201	206	VVQTIE	0.381
204	**T**	202	207	VQTIEV	0.381
205	**I**	203	208	QTIEVN	0.825
206	**E**	204	209	TIEVNS	0.638
207	**V**	205	210	IEVNSF	0.383
208	**N**	206	211	EVNSFS	0.732
209	**S**	207	212	VNSFSG	0.419
210	**F**	208	213	NSFSGY	0.884
211	**S**	209	214	SFSGYL	0.453
212	**G**	210	215	FSGYLK	0.676
213	**Y**	211	216	SGYLKL	0.644
214	**L**	212	217	GYLKLT	0.693
215	**K**	213	218	YLKLTD	1.17
216	**L**	214	219	LKLTDN	1.201
217	**T**	215	220	KLTDNV	1.081
218	**D**	216	221	LTDNVY	0.847
219	**N**	217	222	TDNVYI	0.72
220	**V**	218	223	DNVYIK	0.998
221	**Y**	219	224	NVYIKN	0.961
222	**I**	220	225	VYIKNA	0.603
223	**K**	221	226	YIKNAD	1.358
224	**N**	222	227	IKNADI	0.607
225	**A**	223	228	KNADIV	0.643
226	**D**	224	229	NADIVE	0.557
227	**I**	225	230	ADIVEE	0.6
228	**V**	226	231	DIVEEA	0.6
229	**E**	227	232	IVEEAK	0.718
230	**E**	228	233	VEEAKK	2.049
231	**A**	229	234	EEAKKV	2.049
232	**K**	230	235	EAKKVK	2.366
233	**K**	231	236	AKKVKP	2.113
234	**V**	232	237	KKVKPT	3.018
235	**K**	233	238	KVKPTV	1.12

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236	**P**	234	239	VKPTVV	0.416
237	**T**	235	240	KPTVVV	0.416
238	**V**	236	241	PTVVVN	0.334
239	**V**	237	242	TVVVNA	0.218
240	**V**	238	243	VVVNAA	0.153
241	**N**	239	244	VVNAAN	0.331
242	**A**	240	245	VNAANV	0.331
243	**A**	241	246	NAANVY	0.699
244	**N**	242	247	AANVYL	0.359
245	**V**	243	248	ANVYLK	0.71
246	**Y**	244	249	NVYLKH	0.956
247	**L**	245	250	VYLKHG	0.588
248	**K**	246	251	YLKHGG	0.785
249	**H**	247	252	LKHGGG	0.496
250	**G**	248	253	KHGGGV	0.446
251	**G**	249	254	HGGGVA	0.225
252	**G**	250	255	GGGVAG	0.164
253	**V**	251	256	GGVAGA	0.167
254	**A**	252	257	GVAGAL	0.139
255	**G**	253	258	VAGALN	0.227
256	**A**	254	259	AGALNK	0.61
257	**L**	255	260	GALNKA	0.61
258	**N**	256	261	ALNKAT	0.89
259	**K**	257	262	LNKATN	1.417
260	**A**	258	263	NKATNN	2.763
261	**T**	259	264	KATNNA	1.736
262	**N**	260	265	ATNNAM	0.859
263	**N**	261	266	TNNAMQ	1.472
264	**A**	262	267	NNAMQV	0.757
265	**M**	263	268	NAMQVE	0.815
266	**Q**	264	269	AMQVES	0.68
267	**V**	265	270	MQVESD	1.123
268	**E**	266	271	QVESDD	1.896
269	**S**	267	272	VESDDY	1.715
270	**D**	268	273	ESDDYI	1.62
271	**D**	269	274	SDDYIA	0.945
272	**Y**	270	275	DDYIAT	1.018
273	**I**	271	276	DYIATN	0.98
274	**A**	272	277	YIATNG	0.581
275	**T**	273	278	IATNGP	0.573
276	**N**	274	279	ATNGPL	0.674
277	**G**	275	280	TNGPLK	1.334
278	**P**	276	281	NGPLKV	0.686
279	**L**	277	282	GPLKVG	0.422
280	**K**	278	283	PLKVGG	0.422
281	**V**	279	284	LKVGGS	0.366
282	**G**	280	285	KVGGSC	0.238

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283	**G**	281	286	VGGSCV	0.088
284	**S**	282	287	GGSCVL	0.098
285	**C**	283	288	GSCVLS	0.133
286	**V**	284	289	SCVLSG	0.133
287	**L**	285	290	CVLSGH	0.135
288	**S**	286	291	VLSGHN	0.405
289	**G**	287	292	LSGHNL	0.45
290	**H**	288	293	SGHNLA	0.551
291	**N**	289	294	GHNLAK	0.822
292	**L**	290	295	HNLAKH	1.13
293	**A**	291	296	NLAKHC	0.445
294	**K**	292	297	LAKHCL	0.228
295	**H**	293	298	AKHCLH	0.377
296	**C**	294	299	KHCLHV	0.277
297	**L**	295	300	HCLHVV	0.103
298	**H**	296	301	CLHVVG	0.075
299	**V**	297	302	LHVVGP	0.216
300	**V**	298	303	HVVGPN	0.42
301	**G**	299	304	VVGPNV	0.229
302	**P**	300	305	VGPNVN	0.497
303	**N**	301	306	GPNVNK	1.338
304	**V**	302	307	PNVNKG	1.338
305	**N**	303	308	NVNKGE	1.499
306	**K**	304	309	VNKGED	1.557
307	**G**	305	310	NKGEDI	1.47
308	**E**	306	311	KGEDIQ	1.583
309	**D**	307	312	GEDIQL	0.653
310	**I**	308	313	EDIQLL	0.544
311	**Q**	309	314	DIQLLK	0.628
312	**L**	310	315	IQLLKS	0.504
313	**L**	311	316	QLLKSA	0.727
314	**K**	312	317	LLKSAY	0.657
315	**S**	313	318	LKSAYE	1.38
316	**A**	314	319	KSAYEN	2.692
317	**Y**	315	320	SAYENF	1.166
318	**E**	316	321	AYENFN	1.399
319	**N**	317	322	YENFNQ	2.398
320	**F**	318	323	ENFNQH	2.082
321	**N**	319	324	NFNQHE	2.082
322	**Q**	320	325	FNQHEV	0.961
323	**H**	321	326	NQHEVL	0.915
324	**E**	322	327	QHEVLL	0.469
325	**V**	323	328	HEVLLA	0.274
326	**L**	324	329	EVLLAP	0.311
327	**L**	325	330	VLLAPL	0.148
328	**A**	326	331	LLAPLL	0.165
329	**P**	327	332	LAPLLS	0.268

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330	**L**	328	333	APLLSA	0.328
331	**L**	329	334	PLLSAG	0.321
332	**S**	330	335	LLSAGI	0.146
333	**A**	331	336	LSAGIF	0.153
334	**G**	332	337	SAGIFG	0.183
335	**I**	333	338	AGIFGA	0.138
336	**F**	334	339	GIFGAD	0.228
337	**G**	335	340	IFGADP	0.357
338	**A**	336	341	FGADPI	0.357
339	**D**	337	342	GADPIH	0.561
340	**P**	338	343	ADPIHS	0.76
341	**I**	339	344	DPIHSL	0.62
342	**H**	340	345	PIHSLR	0.727
343	**S**	341	346	IHSLRV	0.349
344	**L**	342	347	HSLRVC	0.267
345	**R**	343	348	SLRVCV	0.146
346	**V**	344	349	LRVCVD	0.181
347	**C**	345	350	RVCVDT	0.318
348	**V**	346	351	VCVDTV	0.12
349	**D**	347	352	CVDTVR	0.318
350	**T**	348	353	VDTVRT	0.855
351	**V**	349	354	DTVRTN	1.853
352	**R**	350	355	TVRTNV	0.823
353	**T**	351	356	VRTNVY	0.894
354	**N**	352	357	RTNVYL	0.993
355	**V**	353	358	TNVYLA	0.512
356	**Y**	354	359	NVYLAV	0.263
357	**L**	355	360	VYLAVF	0.142
358	**A**	356	361	YLAVFD	0.319
359	**V**	357	362	LAVFDK	0.407
360	**F**	358	363	AVFDKN	0.794
361	**D**	359	364	VFDKNL	0.649
362	**K**	360	365	FDKNLY	1.369
363	**N**	361	366	DKNLYD	2.641
364	**L**	362	367	KNLYDK	3.162
365	**Y**	363	368	NLYDKL	1.304
366	**D**	364	369	LYDKLV	0.602
367	**K**	365	370	YDKLVS	0.978
368	**L**	366	371	DKLVSS	0.836
369	**V**	367	372	KLVSSF	0.434
370	**S**	368	373	LVSSFL	0.179
371	**S**	369	374	VSSFLE	0.376
372	**F**	370	375	SSFLEM	0.501
373	**L**	371	376	SFLEMK	0.747
374	**E**	372	377	FLEMKS	0.747
375	**M**	373	378	LEMKSE	1.495
376	**K**	374	379	EMKSEK	3.624

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377	**S**	375	380	MKSEKQ	3.624
378	**E**	376	381	KSEKQV	2.718
379	**K**	377	382	SEKQVE	2.354
380	**Q**	378	383	EKQVEQ	3.042
381	**V**	379	384	KQVEQK	3.513
382	**E**	380	385	QVEQKI	1.231
383	**Q**	381	386	VEQKIA	0.718
384	**K**	382	387	EQKIAE	1.676
385	**I**	383	388	QKIAEI	0.678
386	**A**	384	389	KIAEIP	0.606
387	**E**	385	390	IAEIPK	0.606
388	**I**	386	391	AEIPKE	1.496
389	**P**	387	392	EIPKEE	2.565
390	**K**	388	393	IPKEEV	1.099
391	**E**	389	394	PKEEVK	3.137
392	**E**	390	395	KEEVKP	3.137
393	**V**	391	396	EEVKPF	1.358
394	**K**	392	397	EVKPFI	0.55
395	**P**	393	398	VKPFIT	0.458
396	**F**	394	399	KPFITE	1.069
397	**I**	395	400	PFITES	0.716
398	**T**	396	401	FITESK	0.926
399	**E**	397	402	ITESKP	1.654
400	**S**	398	403	TESKPS	3.162
401	**K**	399	404	ESKPSV	1.626
402	**P**	400	405	SKPSVE	1.626
403	**S**	401	406	KPSVEQ	2.102
404	**V**	402	407	PSVEQR	2.058
405	**E**	403	408	SVEQRK	2.662
406	**Q**	404	409	VEQRKQ	3.44
407	**R**	405	410	EQRKQD	7.741
408	**K**	406	411	QRKQDD	7.465
409	**Q**	407	412	RKQDDK	8.62
410	**D**	408	413	KQDDKK	8.801
411	**D**	409	414	QDDKKI	3.085
412	**K**	410	415	DDKKIK	3.562
413	**K**	411	416	DKKIKA	2.155
414	**I**	412	417	KKIKAC	0.692
415	**K**	413	418	KIKACV	0.257
416	**A**	414	419	IKACVE	0.222
417	**C**	415	420	KACVEE	0.549
418	**V**	416	421	ACVEEV	0.204
419	**E**	417	422	CVEEVT	0.291
420	**E**	418	423	VEEVTT	0.784
421	**V**	419	424	EEVTTT	1.525
422	**T**	420	425	EVTTTL	0.726
423	**T**	421	426	VTTTLE	0.726

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424	**T**	422	427	TTTLEE	1.694
425	**L**	423	428	TTLEET	1.694
426	**E**	424	429	TLEETK	2.347
427	**E**	425	430	LEETKF	1.408
428	**T**	426	431	EETKFL	1.408
429	**K**	427	432	ETKFLT	1.174
430	**F**	428	433	TKFLTE	1.174
431	**L**	429	434	KFLTEN	1.308
432	**T**	430	435	FLTENL	0.539
433	**E**	431	436	LTENLL	0.514
434	**N**	432	437	TENLLL	0.514
435	**L**	433	438	ENLLLY	0.558
436	**L**	434	439	NLLLYI	0.226
437	**L**	435	440	LLLYID	0.234
438	**Y**	436	441	LLYIDI	0.199
439	**I**	437	442	LYIDIN	0.389
440	**D**	438	443	YIDING	0.466
441	**I**	439	444	IDINGN	0.478
442	**N**	440	445	DINGNL	0.563
443	**G**	441	446	INGNLH	0.459
444	**N**	442	447	NGNLHP	1.012
445	**L**	443	448	GNLHPD	1.051
446	**H**	444	449	NLHPDS	1.423
447	**P**	445	450	LHPDSA	0.894
448	**D**	446	451	HPDSAT	1.564
449	**S**	447	452	PDSATL	0.948
450	**A**	448	453	DSATLV	0.455
451	**T**	449	454	SATLVS	0.365
452	**L**	450	455	ATLVSD	0.455
453	**V**	451	456	TLVSDI	0.316
454	**S**	452	457	LVSDID	0.365
455	**D**	453	458	VSDIDI	0.311
456	**I**	454	459	SDIDIT	0.604
457	**D**	455	460	DIDITF	0.39
458	**I**	456	461	IDITFL	0.193
459	**T**	457	462	DITFLK	0.55
460	**F**	458	463	ITFLKK	0.658
461	**L**	459	464	TFLKKD	1.568
462	**K**	460	465	FLKKDA	1.098
463	**K**	461	466	LKKDAP	1.96
464	**D**	462	467	KKDAPY	3.725
465	**A**	463	468	KDAPYI	1.306
466	**P**	464	469	DAPYIV	0.485
467	**Y**	465	470	APYIVG	0.287
468	**I**	466	471	PYIVGD	0.475
469	**V**	467	472	YIVGDV	0.228
470	**G**	468	473	IVGDVV	0.108

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471	**D**	469	474	VGDVVQ	0.267
472	**V**	470	475	GDVVQE	0.622
473	**V**	471	476	DVVQEG	0.622
474	**Q**	472	477	VVQEGV	0.276
475	**E**	473	478	VQEGVL	0.307
476	**G**	474	479	QEGVLT	0.597
477	**V**	475	480	EGVLTA	0.348
478	**L**	476	481	GVLTAV	0.149
479	**T**	477	482	VLTAVV	0.112
480	**A**	478	483	LTAVVI	0.106
481	**V**	479	484	TAVVIP	0.198
482	**V**	480	485	AVVIPT	0.198
483	**I**	481	486	VVIPTK	0.393
484	**P**	482	487	VIPTKK	1.058
485	**T**	483	488	IPTKKA	1.44
486	**K**	484	489	PTKKAG	2.033
487	**K**	485	490	TKKAGG	1.301
488	**A**	486	491	KKAGGT	1.301
489	**G**	487	492	KAGGTT	0.939
490	**G**	488	493	AGGTTE	0.813
491	**T**	489	494	GGTTEM	0.796
492	**T**	490	495	GTTEML	0.664
493	**E**	491	496	TTEMLA	0.678
494	**M**	492	497	TEMLAK	0.939
495	**L**	493	498	EMLAKA	0.657
496	**A**	494	499	MLAKAL	0.313
497	**K**	495	500	LAKALR	0.619
498	**A**	496	501	AKALRK	1.502
499	**L**	497	502	KALRKV	1.104
500	**R**	498	503	ALRKVP	0.853
501	**K**	499	504	LRKVPT	1.219
502	**V**	500	505	RKVPTD	2.468
503	**P**	501	506	KVPTDN	2.027
504	**T**	502	507	VPTDNY	1.588
505	**D**	503	508	PTDNYI	1.5
506	**N**	504	509	TDNYIT	1.4
507	**Y**	505	510	DNYITT	1.4
508	**I**	506	511	NYITTY	1.313
509	**T**	507	512	YITTYP	1.263
510	**T**	508	513	ITTYPG	0.798
511	**Y**	509	514	TTYPGQ	1.97
512	**P**	510	515	TYPGQG	1.351
513	**G**	511	516	YPGQGL	0.772
514	**Q**	512	517	PGQGLN	0.792
515	**G**	513	518	GQGLNG	0.507
516	**L**	514	519	QGLNGY	0.803
517	**N**	515	520	GLNGYT	0.669

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518	**G**	516	521	LNGYTV	0.502
519	**Y**	517	522	NGYTVE	1.054
520	**T**	518	523	GYTVEE	1.135
521	**V**	519	524	YTVEEA	1.159
522	**E**	520	525	TVEEAK	1.479
523	**E**	521	526	VEEAKT	1.479
524	**A**	522	527	EEAKTV	1.479
525	**K**	523	528	EAKTVL	0.704
526	**T**	524	529	AKTVLK	0.813
527	**V**	525	530	KTVLKK	1.61
528	**L**	526	531	TVLKKC	0.431
529	**K**	527	532	VLKKCK	0.598
530	**K**	528	533	LKKCKS	1.08
531	**C**	529	534	KKCKSA	1.322
532	**K**	530	535	KCKSAF	0.573
533	**S**	531	536	CKSAFY	0.449
534	**A**	532	537	KSAFYI	0.587
535	**F**	533	538	SAFYIL	0.242
536	**Y**	534	539	AFYILP	0.279
537	**I**	535	540	FYILPS	0.37
538	**L**	536	541	YILPSI	0.3
539	**P**	537	542	ILPSII	0.134
540	**S**	538	543	LPSIIS	0.256
541	**I**	539	544	PSIISN	0.5
542	**I**	540	545	SIISNE	0.56
543	**S**	541	546	IISNEK	0.836
544	**N**	542	547	ISNEKQ	2.064
545	**E**	543	548	SNEKQE	5.1
546	**K**	544	549	NEKQEI	2.668
547	**Q**	545	550	EKQEIL	1.368
548	**E**	546	551	KQEILG	0.782
549	**I**	547	552	QEILGT	0.564
550	**L**	548	553	EILGTV	0.242
551	**G**	549	554	ILGTVS	0.187
552	**T**	550	555	LGTVSW	0.281
553	**V**	551	556	GTVSWN	0.547
554	**S**	552	557	TVSWNL	0.456
555	**W**	553	558	VSWNLR	0.619
556	**N**	554	559	SWNLRE	1.444
557	**L**	555	560	WNLREM	1.066
558	**R**	556	561	NLREML	0.836
559	**E**	557	562	LREMLA	0.525
560	**M**	558	563	REMLAH	0.867
561	**L**	559	564	EMLAHA	0.447
562	**A**	560	565	MLAHAE	0.447
563	**H**	561	566	LAHAEE	0.783
564	**A**	562	567	AHAEET	1.37

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565	**E**	563	568	HAEETR	2.655
566	**E**	564	569	AEETRK	3.902
567	**T**	565	570	EETRKL	3.186
568	**R**	566	571	ETRKLM	1.82
569	**K**	567	572	TRKLMP	1.625
570	**L**	568	573	RKLMPV	0.836
571	**M**	569	574	KLMPVC	0.229
572	**P**	570	575	LMPVCV	0.085
573	**V**	571	576	MPVCVE	0.178
574	**C**	572	577	PVCVET	0.26
575	**V**	573	578	VCVETK	0.336
576	**E**	574	579	CVETKA	0.458
577	**T**	575	580	VETKAI	0.599
578	**K**	576	581	ETKAIV	0.599
579	**A**	577	582	TKAIVS	0.463
580	**I**	578	583	KAIVST	0.463
581	**V**	579	584	AIVSTI	0.162
582	**S**	580	585	IVSTIQ	0.278
583	**T**	581	586	VSTIQR	0.778
584	**I**	582	587	STIQRK	2.095
585	**Q**	583	588	TIQRKY	2.45
586	**R**	584	589	IQRKYK	3.395
587	**K**	585	590	QRKYKG	4.793
588	**Y**	586	591	RKYKGI	1.94
589	**K**	587	592	KYKGIK	1.981
590	**G**	588	593	YKGIKI	0.694
591	**I**	589	594	KGIKIQ	0.767
592	**K**	590	595	GIKIQE	0.665
593	**I**	591	596	IKIQEG	0.665
594	**Q**	592	597	KIQEGV	0.704
595	**E**	593	598	IQEGVV	0.261
596	**G**	594	599	QEGVVD	0.622
597	**V**	595	600	EGVVDY	0.563
598	**V**	596	601	GVVDYG	0.322
599	**D**	597	602	VVDYGA	0.328
600	**Y**	598	603	VDYGAR	0.866
601	**G**	599	604	DYGARF	1.011
602	**A**	600	605	YGARFY	0.948
603	**R**	601	606	GARFYF	0.524
604	**F**	602	607	ARFYFY	0.83
605	**Y**	603	608	RFYFYT	1.186
606	**F**	604	609	FYFYTS	0.811
607	**Y**	605	610	YFYTSK	1.873
608	**T**	606	611	FYTSKT	1.726
609	**S**	607	612	YTSKTT	2.876
610	**K**	608	613	TSKTTV	1.362
611	**T**	609	614	SKTTVA	0.954

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612	**T**	610	615	KTTVAS	0.954
613	**V**	611	616	TTVASL	0.393
614	**A**	612	617	TVASLI	0.191
615	**S**	613	618	VASLIN	0.213
616	**L**	614	619	ASLINT	0.414
617	**I**	615	620	SLINTL	0.338
618	**N**	616	621	LINTLN	0.405
619	**T**	617	622	INTLND	0.821
620	**L**	618	623	NTLNDL	0.966
621	**N**	619	624	TLNDLN	0.966
622	**D**	620	625	LNDLNE	1.159
623	**L**	621	626	NDLNET	2.028
624	**N**	622	627	DLNETL	1.04
625	**E**	623	628	LNETLV	0.462
626	**T**	624	629	NETLVT	0.809
627	**L**	625	630	ETLVTM	0.498
628	**V**	626	631	TLVTMP	0.444
629	**T**	627	632	LVTMPL	0.254
630	**M**	628	633	VTMPLG	0.305
631	**P**	629	634	TMPLGY	0.643
632	**L**	630	635	MPLGYV	0.331
633	**G**	631	636	PLGYVT	0.483
634	**Y**	632	637	LGYVTH	0.425
635	**V**	633	638	GYVTHG	0.51
636	**T**	634	639	YVTHGL	0.425
637	**H**	635	640	VTHGLN	0.436
638	**G**	636	641	THGLNL	0.484
639	**L**	637	642	HGLNLE	0.581
640	**N**	638	643	GLNLEE	0.74
641	**L**	639	644	LNLEEA	0.755
642	**E**	640	645	NLEEAA	0.925
643	**E**	641	646	LEEAAR	1.126
644	**A**	642	647	EEAARY	2.14
645	**A**	643	648	EAARYM	1.223
646	**R**	644	649	AARYMR	1.383
647	**Y**	645	650	ARYMRS	1.835
648	**M**	646	651	RYMRSL	1.498
649	**R**	647	652	YMRSLK	1.529
650	**S**	648	653	MRSLKV	0.724
651	**L**	649	654	RSLKVP	1.132
652	**K**	650	655	SLKVPA	0.584
653	**V**	651	656	LKVPAT	0.629
654	**P**	652	657	KVPATV	0.566
655	**A**	653	658	VPATVS	0.379
656	**T**	654	659	PATVSV	0.379
657	**V**	655	660	ATVSVS	0.329
658	**S**	656	661	TVSVSS	0.436

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659	**V**	657	662	VSVSSP	0.467
660	**S**	658	663	SVSSPD	1.051
661	**S**	659	664	VSSPDA	0.792
662	**P**	660	665	SSPDAV	0.792
663	**D**	661	666	SPDAVT	0.853
664	**A**	662	667	PDAVTA	0.643
665	**V**	663	668	DAVTAY	0.652
666	**T**	664	669	AVTAYN	0.628
667	**A**	665	670	VTAYNG	0.615
668	**Y**	666	671	TAYNGY	1.298
669	**N**	667	672	AYNGYL	0.742
670	**G**	668	673	YNGYLT	1.06
671	**Y**	669	674	NGYLTS	0.906
672	**L**	670	675	GYLTSS	0.755
673	**T**	671	676	YLTSSS	1.023
674	**S**	672	677	LTSSSK	1.305
675	**S**	673	678	TSSSKT	2.284
676	**S**	674	679	SSSKTP	2.447
677	**K**	675	680	SSKTPE	3.162
678	**T**	676	681	SKTPEE	4.087
679	**P**	677	682	KTPEEH	4.15
680	**E**	678	683	TPEEHF	1.797
681	**E**	679	684	PEEHFI	0.873
682	**H**	680	685	EEHFIE	0.977
683	**F**	681	686	EHFIET	0.815
684	**I**	682	687	HFIETI	0.33
685	**E**	683	688	FIETIS	0.325
686	**T**	684	689	IETISL	0.309
687	**I**	685	690	ETISLA	0.446
688	**S**	686	691	TISLAG	0.255
689	**L**	687	692	ISLAGS	0.236
690	**A**	688	693	SLAGSY	0.529
691	**G**	689	694	LAGSYK	0.789
692	**S**	690	695	AGSYKD	1.597
693	**Y**	691	696	GSYKDW	1.663
694	**K**	692	697	SYKDWS	2.251
695	**D**	693	698	YKDWSY	2.632
696	**W**	694	699	KDWSYS	2.251
697	**S**	695	700	DWSYSG	1.114
698	**Y**	696	701	WSYSGQ	1.155
699	**S**	697	702	SYSGQS	1.473
700	**G**	698	703	YSGQST	1.586
701	**Q**	699	704	SGQSTQ	1.753
702	**S**	700	705	GQSTQL	1.079
703	**T**	701	706	QSTQLG	1.079
704	**Q**	702	707	STQLGI	0.437
705	**L**	703	708	TQLGIE	0.564

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706	**G**	704	709	QLGIEF	0.339
707	**I**	705	710	LGIEFL	0.161
708	**E**	706	711	GIEFLK	0.391
709	**F**	707	712	IEFLKR	0.774
710	**L**	708	713	EFLKRG	1.092
711	**K**	709	714	FLKRGD	1.053
712	**R**	710	715	LKRGDK	2.432
713	**G**	711	716	KRGDKS	3.953
714	**D**	712	717	RGDKSV	1.467
715	**K**	713	718	GDKSVY	1.174
716	**S**	714	719	DKSVYY	1.858
717	**V**	715	720	KSVYYT	1.606
718	**Y**	716	721	SVYYTS	1.076
719	**Y**	717	722	VYYTSN	1.291
720	**T**	718	723	YYTSNP	2.69
721	**S**	719	724	YTSNPT	2.478
722	**N**	720	725	TSNPTT	2.282
723	**P**	721	726	SNPTTF	1.369
724	**T**	722	727	NPTTFH	1.39
725	**T**	723	728	PTTFHL	0.713
726	**F**	724	729	TTFHLD	0.77
727	**H**	725	730	TFHLDG	0.528
728	**L**	726	731	FHLDGE	0.634
729	**D**	727	732	HLDGEV	0.543
730	**G**	728	733	LDGEVI	0.28
731	**E**	729	734	DGEVIT	0.49
732	**V**	730	735	GEVITF	0.254
733	**I**	731	736	EVITFD	0.428
734	**T**	732	737	VITFDN	0.398
735	**F**	733	738	ITFDNL	0.442
736	**D**	734	739	TFDNLK	1.261
737	**N**	735	740	FDNLKT	1.261
738	**L**	736	741	DNLKTL	1.201
739	**K**	737	742	NLKTLL	0.593
740	**T**	738	743	LKTLLS	0.494
741	**L**	739	744	KTLLSL	0.494
742	**L**	740	745	TLLSLR	0.484
743	**S**	741	746	LLSLRE	0.581
744	**L**	742	747	LSLREV	0.523
745	**R**	743	748	SLREVR	1.242
746	**E**	744	749	LREVRT	1.337
747	**V**	745	750	REVRTI	1.137
748	**R**	746	751	EVRTIK	1.16
749	**T**	747	752	VRTIKV	0.497
750	**I**	748	753	RTIKVF	0.58
751	**K**	749	754	TIKVFT	0.428
752	**V**	750	755	IKVFTT	0.428

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753	**F**	751	756	KVFTTV	0.453
754	**T**	752	757	VFTTVD	0.378
755	**T**	753	758	FTTVDN	0.819
756	**V**	754	759	TTVDNI	0.663
757	**D**	755	760	TVDNIN	0.739
758	**N**	756	761	VDNINL	0.422
759	**I**	757	762	DNINLH	0.774
760	**N**	758	763	NINLHT	0.669
761	**L**	759	764	INLHTQ	0.72
762	**H**	760	765	NLHTQV	0.763
763	**T**	761	766	LHTQVV	0.352
764	**Q**	762	767	HTQVVD	0.713
765	**V**	763	768	TQVVDM	0.518
766	**V**	764	769	QVVDMS	0.481
767	**D**	765	770	VVDMSM	0.275
768	**M**	766	771	VDMSMT	0.535
769	**S**	767	772	DMSMTY	1.129
770	**M**	768	773	MSMTYG	0.669
771	**T**	769	774	SMTYGQ	1.171
772	**Y**	770	775	MTYGQQ	1.513
773	**G**	771	776	TYGQQF	1.324
774	**Q**	772	777	YGQQFG	0.908
775	**Q**	773	778	GQQFGP	0.896
776	**F**	774	779	QQFGPT	1.307
777	**G**	775	780	QFGPTY	1.182
778	**P**	776	781	FGPTYL	0.563
779	**T**	777	782	GPTYLD	1.086
780	**Y**	778	783	PTYLDG	1.086
781	**L**	779	784	TYLDGA	0.709
782	**D**	780	785	YLDGAD	0.821
783	**G**	781	786	LDGADV	0.389
784	**A**	782	787	DGADVT	0.68
785	**D**	783	788	GADVTK	0.815
786	**V**	784	789	ADVTKI	0.577
787	**T**	785	790	DVTKIK	1.143
788	**K**	786	791	VTKIKP	1.058
789	**I**	787	792	TKIKPH	1.94
790	**K**	788	793	KIKPHN	2.161
791	**P**	789	794	IKPHNS	1.448
792	**H**	790	795	KPHNSH	2.811
793	**N**	791	796	PHNSHE	2.435
794	**S**	792	797	HNSHEG	1.558
795	**H**	793	798	NSHEGK	2.29
796	**E**	794	799	SHEGKT	2.055
797	**G**	795	800	HEGKTF	1.328
798	**K**	796	801	EGKTFY	1.529
799	**T**	797	802	GKTFYV	0.655

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800	**F**	798	803	KTFYVL	0.546
801	**Y**	799	804	TFYVLP	0.422
802	**V**	800	805	FYVLPN	0.471
803	**L**	801	806	YVLPND	0.907
804	**P**	802	807	VLPNDD	0.967
805	**N**	803	808	LPNDDT	1.88
806	**D**	804	809	PNDDTL	1.88
807	**D**	805	810	NDDTLR	2.382
808	**T**	806	811	DDTLRV	1.099
809	**L**	807	812	DTLRVE	1.14
810	**R**	808	813	TLRVEA	0.69
811	**V**	809	814	LRVEAF	0.414
812	**E**	810	815	RVEAFE	0.869
813	**A**	811	816	VEAFEY	0.695
814	**F**	812	817	EAFEYY	1.468
815	**E**	813	818	AFEYYH	1.153
816	**Y**	814	819	FEYYHT	1.647
817	**Y**	815	820	EYYHTT	2.746
818	**H**	816	821	YYHTTD	2.647
819	**T**	817	822	YHTTDP	2.613
820	**T**	818	823	HTTDPS	2.235
821	**D**	819	824	TTDPSF	1.422
822	**P**	820	825	TDPSFL	0.813
823	**S**	821	826	DPSFLG	0.557
824	**F**	822	827	PSFLGR	0.653
825	**L**	823	828	SFLGRY	0.662
826	**G**	824	829	FLGRYM	0.489
827	**R**	825	830	LGRYMS	0.757
828	**Y**	826	831	GRYMSA	0.927
829	**M**	827	832	RYMSAL	0.773
830	**S**	828	833	YMSALN	0.634
831	**A**	829	834	MSALNH	0.551
832	**L**	830	835	SALNHT	0.803
833	**N**	831	836	ALNHTK	1.199
834	**H**	832	837	LNHTKK	2.373
835	**T**	833	838	NHTKKW	3.026
836	**K**	834	839	HTKKWK	3.763
837	**K**	835	840	TKKWKY	4.333
838	**W**	836	841	KKWKYP	4.642
839	**K**	837	842	KWKYPQ	4.02
840	**Y**	838	843	WKYPQV	1.492
841	**P**	839	844	KYPQVN	2.282
842	**Q**	840	845	YPQVNG	1.129
843	**V**	841	846	PQVNGL	0.594
844	**N**	842	847	QVNGLT	0.555
845	**G**	843	848	VNGLTS	0.429
846	**L**	844	849	NGLTSI	0.405

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847	**T**	845	850	GLTSIK	0.504
848	**S**	846	851	LTSIKW	0.536
849	**I**	847	852	TSIKWA	0.656
850	**K**	848	853	SIKWAD	0.759
851	**W**	849	854	IKWADN	0.911
852	**A**	850	855	KWADNN	2.09
853	**D**	851	856	WADNNC	0.56
854	**N**	852	857	ADNNCY	0.835
855	**N**	853	858	DNNCYL	0.682
856	**C**	854	859	NNCYLA	0.412
857	**Y**	855	860	NCYLAT	0.37
858	**L**	856	861	CYLATA	0.232
859	**A**	857	862	YLATAL	0.358
860	**T**	858	863	LATALL	0.188
861	**A**	859	864	ATALLT	0.329
862	**L**	860	865	TALLTL	0.269
863	**L**	861	866	ALLTLQ	0.323
864	**T**	862	867	LLTLQQ	0.553
865	**L**	863	868	LTLQQI	0.47
866	**Q**	864	869	TLQQIE	0.987
867	**Q**	865	870	LQQIEL	0.564
868	**I**	866	871	QQIELK	1.368
869	**E**	867	872	QIELKF	0.684
870	**L**	868	873	IELKFN	0.635
871	**K**	869	874	ELKFNP	1.401
872	**F**	870	875	LKFNPP	1.251
873	**N**	871	876	KFNPPA	1.533
874	**P**	872	877	FNPPAL	0.632
875	**P**	873	878	NPPALQ	1.264
876	**A**	874	879	PPALQD	1.313
877	**L**	875	880	PALQDA	0.858
878	**Q**	876	881	ALQDAY	0.869
879	**D**	877	882	LQDAYY	1.348
880	**A**	878	883	QDAYYR	3.201
881	**Y**	879	884	DAYYRA	1.867
882	**Y**	880	885	AYYRAR	2.19
883	**R**	881	886	YYRARA	2.19
884	**A**	882	887	YRARAG	1.383
885	**R**	883	888	RARAGE	1.529
886	**A**	884	889	ARAGEA	0.789
887	**G**	885	890	RAGEAA	0.789
888	**E**	886	891	AGEAAN	0.647
889	**A**	887	892	GEAANF	0.555
890	**A**	888	893	EAANFC	0.301
891	**N**	889	894	AANFCA	0.175
892	**F**	890	895	ANFCAL	0.143
893	**C**	891	896	NFCALI	0.099

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894	**A**	892	897	FCALIL	0.051
895	**L**	893	898	CALILA	0.059
896	**I**	894	899	ALILAY	0.174
897	**L**	895	900	LILAYC	0.092
898	**A**	896	901	ILAYCN	0.18
899	**Y**	897	902	LAYCNK	0.513
900	**C**	898	903	AYCNKT	0.897
901	**N**	899	904	YCNKTV	0.659
902	**K**	900	905	CNKTVG	0.416
903	**T**	901	906	NKTVGE	1.345
904	**V**	902	907	KTVGEL	0.69
905	**G**	903	908	TVGELG	0.341
906	**E**	904	909	VGELGD	0.395
907	**L**	905	910	GELGDV	0.395
908	**G**	906	911	ELGDVR	0.782
909	**D**	907	912	LGDVRE	0.782
910	**V**	908	913	GDVRET	1.368
911	**R**	909	914	DVRETM	1.368
912	**E**	910	915	VRETMS	1.098
913	**T**	911	916	RETMSY	2.318
914	**M**	912	917	ETMSYL	0.976
915	**S**	913	918	TMSYLF	0.488
916	**Y**	914	919	MSYLFQ	0.586
917	**L**	915	920	SYLFQH	0.805
918	**F**	916	921	YLFQHA	0.607
919	**Q**	917	922	LFQHAN	0.623
920	**H**	918	923	FQHANL	0.623
921	**A**	919	924	QHANLD	1.201
922	**N**	920	925	HANLDS	0.93
923	**L**	921	926	ANLDSC	0.366
924	**D**	922	927	NLDSCK	0.725
925	**S**	923	928	LDSCKR	0.883
926	**C**	924	929	DSCKRV	0.795
927	**K**	925	930	SCKRVL	0.392
928	**R**	926	931	CKRVLN	0.471
929	**V**	927	932	KRVLNV	0.652
930	**L**	928	933	RVLNVV	0.242
931	**N**	929	934	VLNVVC	0.066
932	**V**	930	935	LNVVCK	0.178
933	**V**	931	936	NVVCKT	0.312
934	**C**	932	937	VVCKTC	0.104
935	**K**	933	938	VCKTCG	0.139
936	**T**	934	939	CKTCGQ	0.324
937	**C**	935	940	KTCGQQ	1.046
938	**G**	936	941	TCGQQQ	0.906
939	**Q**	937	942	CGQQQT	0.906
940	**Q**	938	943	GQQQTT	2.439

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941	**Q**	939	944	QQQTTL	2.033
942	**T**	940	945	QQTTLK	2.347
943	**T**	941	946	QTTLKG	1.341
944	**L**	942	947	TTLKGV	0.575
945	**K**	943	948	TLKGVE	0.69
946	**G**	944	949	LKGVEA	0.483
947	**V**	945	950	KGVEAV	0.435
948	**E**	946	951	GVEAVM	0.215
949	**A**	947	952	VEAVMY	0.341
950	**V**	948	953	EAVMYM	0.454
951	**M**	949	954	AVMYMG	0.259
952	**Y**	950	955	VMYMGT	0.371
953	**M**	951	956	MYMGTL	0.412
954	**G**	952	957	YMGTLS	0.558
955	**T**	953	958	MGTLSY	0.558
956	**L**	954	959	GTLSYE	0.976
957	**S**	955	960	TLSYEQ	1.708
958	**Y**	956	961	LSYEQF	1.025
959	**E**	957	962	SYEQFK	2.485
960	**Q**	958	963	YEQFKK	3.708
961	**F**	959	964	EQFKKG	2.342
962	**K**	960	965	QFKKGV	1.004
963	**K**	961	966	FKKGVQ	1.004
964	**G**	962	967	KKGVQI	0.813
965	**V**	963	968	KGVQIP	0.628
966	**Q**	964	969	GVQIPC	0.168
967	**I**	965	970	VQIPCT	0.246
968	**P**	966	971	QIPCTC	0.177
969	**C**	967	972	IPCTCG	0.101
970	**T**	968	973	PCTCGK	0.289
971	**C**	969	974	CTCGKQ	0.324
972	**G**	970	975	TCGKQA	0.61
973	**K**	971	976	CGKQAT	0.61
974	**Q**	972	977	GKQATK	2.277
975	**A**	973	978	KQATKY	3.605
976	**T**	974	979	QATKYL	1.487
977	**K**	975	980	ATKYLV	0.637
978	**Y**	976	981	TKYLVQ	1.092
979	**L**	977	982	KYLVQQ	1.311
980	**V**	978	983	YLVQQE	1.135
981	**Q**	979	984	LVQQES	0.971
982	**Q**	980	985	VQQESP	1.82
983	**E**	981	986	QQESPF	2.123
984	**S**	982	987	QESPFV	0.91
985	**P**	983	988	ESPFVM	0.52
986	**F**	984	989	SPFVMM	0.297
987	**V**	985	990	PFVMMS	0.297

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988	**M**	986	991	FVMMSA	0.194
989	**M**	987	992	VMMSAP	0.347
990	**S**	988	993	MMSAPP	0.722
991	**A**	989	994	MSAPPA	0.737
992	**P**	990	995	SAPPAQ	1.29
993	**P**	991	996	APPAQY	1.509
994	**A**	992	997	PPAQYE	2.586
995	**Q**	993	998	PAQYEL	1.379
996	**Y**	994	999	AQYELK	1.784
997	**E**	995	1000	QYELKH	2.403
998	**L**	996	1001	YELKHG	1.373
999	**K**	997	1002	ELKHGT	1.265
1000	**H**	998	1003	LKHGTF	0.632
1001	**G**	999	1004	KHGTFT	1.107
1002	**T**	1000	1005	HGTFTC	0.297
1003	**F**	1001	1006	GTFTCA	0.22
1004	**T**	1002	1007	TFTCAS	0.298
1005	**C**	1003	1008	FTCASE	0.358
1006	**A**	1004	1009	TCASEY	0.648
1007	**S**	1005	1010	CASEYT	0.648
1008	**E**	1006	1011	ASEYTG	1.195
1009	**Y**	1007	1012	SEYTGN	1.903
1010	**T**	1008	1013	EYTGNY	2.225
1011	**G**	1009	1014	YTGNYQ	2.225
1012	**N**	1010	1015	TGNYQC	0.761
1013	**Y**	1011	1016	GNYQCG	0.522
1014	**Q**	1012	1017	NYQCGH	0.718
1015	**C**	1013	1018	YQCGHY	0.699
1016	**G**	1014	1019	QCGHYK	0.892
1017	**H**	1015	1020	CGHYKH	0.701
1018	**Y**	1016	1021	GHYKHI	0.917
1019	**K**	1017	1022	HYKHIT	1.337
1020	**H**	1018	1023	YKHITS	1.317
1021	**I**	1019	1024	KHITSK	1.681
1022	**T**	1020	1025	HITSKE	1.456
1023	**S**	1021	1026	ITSKET	1.544
1024	**K**	1022	1027	TSKETL	1.816
1025	**E**	1023	1028	SKETLY	1.972
1026	**T**	1024	1029	KETLYC	0.789
1027	**L**	1025	1030	ETLYCI	0.276
1028	**Y**	1026	1031	TLYCID	0.267
1029	**C**	1027	1032	LYCIDG	0.183
1030	**I**	1028	1033	YCIDGA	0.224
1031	**D**	1029	1034	CIDGAL	0.118
1032	**G**	1030	1035	IDGALL	0.181
1033	**A**	1031	1036	DGALLT	0.373
1034	**L**	1032	1037	GALLTK	0.447

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1035	**L**	1033	1038	ALLTKS	0.605
1036	**T**	1034	1039	LLTKSS	0.803
1037	**K**	1035	1040	LTKSSE	1.687
1038	**S**	1036	1041	TKSSEY	3.205
1039	**S**	1037	1042	KSSEYK	4.441
1040	**E**	1038	1043	SSEYKG	2.197
1041	**Y**	1039	1044	SEYKGP	2.536
1042	**K**	1040	1045	EYKGPI	1.326
1043	**G**	1041	1046	YKGPIT	1.105
1044	**P**	1042	1047	KGPITD	1.178
1045	**I**	1043	1048	GPITDV	0.437
1046	**T**	1044	1049	PITDVF	0.383
1047	**D**	1045	1050	ITDVFY	0.388
1048	**V**	1046	1051	TDVFYK	1.106
1049	**F**	1047	1052	DVFYKE	1.327
1050	**Y**	1048	1053	VFYKEN	1.278
1051	**K**	1049	1054	FYKENS	2.307
1052	**E**	1050	1055	YKENSY	4.175
1053	**N**	1051	1056	KENSYT	3.846
1054	**S**	1052	1057	ENSYTT	2.775
1055	**Y**	1053	1058	NSYTTT	2.313
1056	**T**	1054	1059	SYTTTI	1.008
1057	**T**	1055	1060	YTTTIK	1.504
1058	**T**	1056	1061	TTTIKP	1.485
1059	**I**	1057	1062	TTIKPV	0.763
1060	**K**	1058	1063	TIKPVT	0.763
1061	**P**	1059	1064	IKPVTY	0.829
1062	**V**	1060	1065	KPVTYK	2.365
1063	**T**	1061	1066	PVTYKL	0.975
1064	**Y**	1062	1067	VTYKLD	1.053
1065	**K**	1063	1068	TYKLDG	1.404
1066	**L**	1064	1069	YKLDGV	0.722
1067	**D**	1065	1070	KLDGVV	0.342
1068	**G**	1066	1071	LDGVVC	0.092
1069	**V**	1067	1072	DGVVCT	0.16
1070	**V**	1068	1073	GVVCTE	0.166
1071	**C**	1069	1074	VVCTEI	0.118
1072	**T**	1070	1075	VCTEID	0.265
1073	**E**	1071	1076	CTEIDP	0.553
1074	**I**	1072	1077	TEIDPK	2.061
1075	**D**	1073	1078	EIDPKL	1.178
1076	**P**	1074	1079	IDPKLD	1.136
1077	**K**	1075	1080	DPKLDN	2.606
1078	**L**	1076	1081	PKLDNY	2.445
1079	**D**	1077	1082	KLDNYY	2.478
1080	**N**	1078	1083	LDNYYK	2.478
1081	**Y**	1079	1084	DNYYKK	6.008

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1082	**Y**	1080	1085	NYYKKD	6.008
1083	**K**	1081	1086	YYKKDN	6.008
1084	**K**	1082	1087	YKKDNS	5.138
1085	**D**	1083	1088	KKDNSY	5.138
1086	**N**	1084	1089	KDNSYF	2.225
1087	**S**	1085	1090	DNSYFT	1.606
1088	**Y**	1086	1091	NSYFTE	1.665
1089	**F**	1087	1092	SYFTEQ	1.793
1090	**T**	1088	1093	YFTEQP	2.069
1091	**E**	1089	1094	FTEQPI	0.926
1092	**Q**	1090	1095	TEQPID	1.785
1093	**P**	1091	1096	EQPIDL	1.02
1094	**I**	1092	1097	QPIDLV	0.437
1095	**D**	1093	1098	PIDLVP	0.39
1096	**L**	1094	1099	IDLVPN	0.406
1097	**V**	1095	1100	DLVPNQ	1.003
1098	**P**	1096	1101	LVPNQP	0.929
1099	**N**	1097	1102	VPNQPY	1.764
1100	**Q**	1098	1103	PNQPYP	3.676
1101	**P**	1099	1104	NQPYPN	3.823
1102	**Y**	1100	1105	QPYPNA	2.402
1103	**P**	1101	1106	PYPNAS	1.858
1104	**N**	1102	1107	YPNASF	1.041
1105	**A**	1103	1108	PNASFD	1.109
1106	**S**	1104	1109	NASFDN	1.153
1107	**F**	1105	1110	ASFDNF	0.621
1108	**D**	1106	1111	SFDNFK	1.23
1109	**N**	1107	1112	FDNFKF	0.794
1110	**F**	1108	1113	DNFKFV	0.681
1111	**K**	1109	1114	NFKFVC	0.219
1112	**F**	1110	1115	FKFVCD	0.227
1113	**V**	1111	1116	KFVCDN	0.422
1114	**C**	1112	1117	FVCDNI	0.148
1115	**D**	1113	1118	VCDNIK	0.341
1116	**N**	1114	1119	CDNIKF	0.398
1117	**I**	1115	1120	DNIKFA	0.75
1118	**K**	1116	1121	NIKFAD	0.75
1119	**F**	1117	1122	IKFADD	0.779
1120	**A**	1118	1123	KFADDL	0.917
1121	**D**	1119	1124	FADDLN	0.737
1122	**D**	1120	1125	ADDLNQ	1.474
1123	**L**	1121	1126	DDLNQL	1.204
1124	**N**	1122	1127	DLNQLT	1.04
1125	**Q**	1123	1128	LNQLTG	0.616
1126	**L**	1124	1129	NQLTGY	1.171
1127	**T**	1125	1130	QLTGYK	1.456
1128	**G**	1126	1131	LTGYKK	1.682

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1129	**Y**	1127	1132	TGYKKP	3.153
1130	**K**	1128	1133	GYKKPA	2.207
1131	**K**	1129	1134	YKKPAS	2.989
1132	**P**	1130	1135	KKPASR	3.736
1133	**A**	1131	1136	KPASRE	3.235
1134	**S**	1132	1137	PASREL	1.334
1135	**R**	1133	1138	ASRELK	1.726
1136	**E**	1134	1139	SRELKV	1.268
1137	**L**	1135	1140	RELKVT	1.365
1138	**K**	1136	1141	ELKVTF	0.604
1139	**V**	1137	1142	LKVTFF	0.302
1140	**T**	1138	1143	KVTFFP	0.566
1141	**F**	1139	1144	VTFFPD	0.473
1142	**F**	1140	1145	TFFPDL	0.525
1143	**P**	1141	1146	FFPDLN	0.585
1144	**D**	1142	1147	FPDLNG	0.669
1145	**L**	1143	1148	PDLNGD	1.289
1146	**N**	1144	1149	DLNGDV	0.619
1147	**G**	1145	1150	LNGDVV	0.275
1148	**D**	1146	1151	NGDVVA	0.337
1149	**V**	1147	1152	GDVVAI	0.147
1150	**V**	1148	1153	DVVAID	0.248
1151	**A**	1149	1154	VVAIDY	0.233
1152	**I**	1150	1155	VAIDYK	0.627
1153	**D**	1151	1156	AIDYKH	1.149
1154	**Y**	1152	1157	IDYKHY	1.782
1155	**K**	1153	1158	DYKHYT	3.669
1156	**H**	1154	1159	YKHYTP	3.397
1157	**Y**	1155	1160	KHYTPS	2.905
1158	**T**	1156	1161	HYTPSF	1.258
1159	**P**	1157	1162	YTPSFK	1.849
1160	**S**	1158	1163	TPSFKK	2.36
1161	**F**	1159	1164	PSFKKG	1.618
1162	**K**	1160	1165	SFKKGA	1.057
1163	**K**	1161	1166	FKKGAK	1.578
1164	**G**	1162	1167	KKGAKL	1.502
1165	**A**	1163	1168	KGAKLL	0.62
1166	**K**	1164	1169	GAKLLH	0.422
1167	**L**	1165	1170	AKLLHK	0.852
1168	**L**	1166	1171	KLLHKP	1.304
1169	**H**	1167	1172	LLHKPI	0.457
1170	**K**	1168	1173	LHKPIV	0.411
1171	**P**	1169	1174	HKPIVW	0.524
1172	**I**	1170	1175	KPIVWH	0.524
1173	**V**	1171	1176	PIVWHV	0.195
1174	**W**	1172	1177	IVWHVN	0.202
1175	**H**	1173	1178	VWHVNN	0.464

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1176	**V**	1174	1179	WHVNNA	0.632
1177	**N**	1175	1180	HVNNAT	0.868
1178	**N**	1176	1181	VNNATN	1.025
1179	**A**	1177	1182	NNATNK	2.763
1180	**T**	1178	1183	NATNKA	1.736
1181	**N**	1179	1184	ATNKAT	1.558
1182	**K**	1180	1185	TNKATY	2.416
1183	**A**	1181	1186	NKATYK	3.348
1184	**T**	1182	1187	KATYKP	3.219
1185	**Y**	1183	1188	ATYKPN	2.588
1186	**K**	1184	1189	TYKPNT	3.698
1187	**P**	1185	1190	YKPNTW	2.694
1188	**N**	1186	1191	KPNTWC	0.922
1189	**T**	1187	1192	PNTWCI	0.323
1190	**W**	1188	1193	NTWCIR	0.409
1191	**C**	1189	1194	TWCIRC	0.136
1192	**I**	1190	1195	WCIRCL	0.078
1193	**R**	1191	1196	CIRCLW	0.078
1194	**C**	1192	1197	IRCLWS	0.195
1195	**L**	1193	1198	RCLWST	0.401
1196	**W**	1194	1199	CLWSTK	0.41
1197	**S**	1195	1200	LWSTKP	1.182
1198	**T**	1196	1201	WSTKPV	1.063
1199	**K**	1197	1202	STKPVE	1.751
1200	**P**	1198	1203	TKPVET	1.886
1201	**V**	1199	1204	KPVETS	1.751
1202	**E**	1200	1205	PVETSN	1.408
1203	**T**	1201	1206	VETSNS	1.221
1204	**S**	1202	1207	ETSNSF	1.424
1205	**N**	1203	1208	TSNSFD	1.373
1206	**S**	1204	1209	SNSFDV	0.706
1207	**F**	1205	1210	NSFDVL	0.435
1208	**D**	1206	1211	SFDVLK	0.54
1209	**V**	1207	1212	FDVLKS	0.54
1210	**L**	1208	1213	DVLKSE	1.081
1211	**K**	1209	1214	VLKSED	1.081
1212	**S**	1210	1215	LKSEDA	1.471
1213	**E**	1211	1216	KSEDAQ	3.09
1214	**D**	1212	1217	SEDAQG	1.529
1215	**A**	1213	1218	EDAQGM	1.129
1216	**Q**	1214	1219	DAQGMD	1.089
1217	**G**	1215	1220	AQGMDN	1.048
1218	**M**	1216	1221	QGMDNL	0.856
1219	**D**	1217	1222	GMDNLA	0.499
1220	**N**	1218	1223	MDNLAC	0.27
1221	**L**	1219	1224	DNLACE	0.473
1222	**A**	1220	1225	NLACED	0.473

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1223	**C**	1221	1226	LACEDL	0.243
1224	**E**	1222	1227	ACEDLK	0.589
1225	**D**	1223	1228	CEDLKP	0.901
1226	**L**	1224	1229	EDLKPV	1.247
1227	**K**	1225	1230	DLKPVS	0.965
1228	**P**	1226	1231	LKPVSE	1.001
1229	**V**	1227	1232	KPVSEE	2.102
1230	**S**	1228	1233	PVSEEV	0.78
1231	**E**	1229	1234	VSEEVV	0.374
1232	**E**	1230	1235	SEEVVE	0.874
1233	**V**	1231	1236	EEVVEN	1.048
1234	**V**	1232	1237	EVVENP	0.936
1235	**E**	1233	1238	VVENPT	0.78
1236	**N**	1234	1239	VENPTI	0.737
1237	**P**	1235	1240	ENPTIQ	1.719
1238	**T**	1236	1241	NPTIQK	1.985
1239	**I**	1237	1242	PTIQKD	2.061
1240	**Q**	1238	1243	TIQKDV	0.989
1241	**K**	1239	1244	IQKDVL	0.565
1242	**D**	1240	1245	QKDVLE	1.397
1243	**V**	1241	1246	KDVLEC	0.432
1244	**L**	1242	1247	DVLECN	0.348
1245	**E**	1243	1248	VLECNV	0.155
1246	**C**	1244	1249	LECNVK	0.416
1247	**N**	1245	1250	ECNVKT	0.729
1248	**V**	1246	1251	CNVKTT	0.607
1249	**K**	1247	1252	NVKTTE	1.962
1250	**T**	1248	1253	VKTTEV	0.905
1251	**T**	1249	1254	KTTEVV	0.905
1252	**E**	1250	1255	TTEVVG	0.448
1253	**V**	1251	1256	TEVVGD	0.518
1254	**V**	1252	1257	EVVGDI	0.252
1255	**G**	1253	1258	VVGDII	0.102
1256	**D**	1254	1259	VGDIIL	0.113
1257	**I**	1255	1260	GDIILK	0.305
1258	**I**	1256	1261	DIILKP	0.477
1259	**L**	1257	1262	IILKPA	0.288
1260	**K**	1258	1263	ILKPAN	0.662
1261	**P**	1259	1264	LKPANN	1.518
1262	**A**	1260	1265	KPANNS	2.467
1263	**N**	1261	1266	PANNSL	1.017
1264	**N**	1262	1267	ANNSLK	1.316
1265	**S**	1263	1268	NNSLKI	0.913
1266	**L**	1264	1269	NSLKIT	0.819
1267	**K**	1265	1270	SLKITE	0.882
1268	**I**	1266	1271	LKITEE	1.14
1269	**T**	1267	1272	KITEEV	1.026

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1270	**E**	1268	1273	ITEEVG	0.508
1271	**E**	1269	1274	TEEVGH	0.986
1272	**V**	1270	1275	EEVGHT	0.986
1273	**G**	1271	1276	EVGHTD	0.95
1274	**H**	1272	1277	VGHTDL	0.453
1275	**T**	1273	1278	GHTDLM	0.603
1276	**D**	1274	1279	HTDLMA	0.616
1277	**L**	1275	1280	TDLMAA	0.457
1278	**M**	1276	1281	DLMAAY	0.497
1279	**A**	1277	1282	LMAAYV	0.221
1280	**A**	1278	1283	MAAYVD	0.447
1281	**Y**	1279	1284	AAYVDN	0.726
1282	**V**	1280	1285	AYVDNS	0.963
1283	**D**	1281	1286	YVDNSS	1.278
1284	**N**	1282	1287	VDNSSL	0.673
1285	**S**	1283	1288	DNSSLT	1.308
1286	**S**	1284	1289	NSSLTI	0.549
1287	**L**	1285	1290	SSLTIK	0.683
1288	**T**	1286	1291	SLTIKK	1.019
1289	**I**	1287	1292	LTIKKP	1.176
1290	**K**	1288	1293	TIKKPN	2.292
1291	**K**	1289	1294	IKKPNE	2.751
1292	**P**	1290	1295	KKPNEL	3.236
1293	**N**	1291	1296	KPNELS	2.169
1294	**E**	1292	1297	PNELSR	2.124
1295	**L**	1293	1298	NELSRV	1.019
1296	**S**	1294	1299	ELSRVL	0.523
1297	**R**	1295	1300	LSRVLG	0.299
1298	**V**	1296	1301	SRVLGL	0.299
1299	**L**	1297	1302	RVLGLK	0.446
1300	**G**	1298	1303	VLGLKT	0.328
1301	**L**	1299	1304	LGLKTL	0.365
1302	**K**	1300	1305	GLKTLA	0.447
1303	**T**	1301	1306	LKTLAT	0.652
1304	**L**	1302	1307	KTLATH	1.076
1305	**A**	1303	1308	TLATHG	0.532
1306	**T**	1304	1309	LATHGL	0.304
1307	**H**	1305	1310	ATHGLA	0.373
1308	**G**	1306	1311	THGLAA	0.373
1309	**L**	1307	1312	HGLAAV	0.192
1310	**A**	1308	1313	GLAAVN	0.227
1311	**A**	1309	1314	LAAVNS	0.307
1312	**V**	1310	1315	AAVNSV	0.276
1313	**N**	1311	1316	AVNSVP	0.423
1314	**S**	1312	1317	VNSVPW	0.44
1315	**V**	1313	1318	NSVPWD	0.989
1316	**P**	1314	1319	SVPWDT	0.888

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1317	**W**	1315	1320	VPWDTI	0.464
1318	**D**	1316	1321	PWDTIA	0.632
1319	**T**	1317	1322	WDTIAN	0.658
1320	**I**	1318	1323	DTIANY	0.98
1321	**A**	1319	1324	TIANYA	0.593
1322	**N**	1320	1325	IANYAK	0.821
1323	**Y**	1321	1326	ANYAKP	1.812
1324	**A**	1322	1327	NYAKPF	1.553
1325	**K**	1323	1328	YAKPFL	0.796
1326	**P**	1324	1329	AKPFLN	0.817
1327	**F**	1325	1330	KPFLNK	1.618
1328	**L**	1326	1331	PFLNKV	0.601
1329	**N**	1327	1332	FLNKVV	0.288
1330	**K**	1328	1333	LNKVVS	0.446
1331	**V**	1329	1334	NKVVST	0.781
1332	**V**	1330	1335	KVVSTT	0.701
1333	**S**	1331	1336	VVSTTT	0.506
1334	**T**	1332	1337	VSTTTN	1.095
1335	**T**	1333	1338	STTTNI	1.035
1336	**T**	1334	1339	TTTNIV	0.573
1337	**N**	1335	1340	TTNIVT	0.573
1338	**I**	1336	1341	TNIVTR	0.778
1339	**V**	1337	1342	NIVTRC	0.289
1340	**T**	1338	1343	IVTRCL	0.148
1341	**R**	1339	1344	VTRCLN	0.34
1342	**C**	1340	1345	TRCLNR	0.897
1343	**L**	1341	1346	RCLNRV	0.461
1344	**N**	1342	1347	CLNRVC	0.126
1345	**R**	1343	1348	LNRVCT	0.34
1346	**V**	1344	1349	NRVCTN	0.663
1347	**C**	1345	1350	RVCTNY	0.646
1348	**T**	1346	1351	VCTNYM	0.326
1349	**N**	1347	1352	CTNYMP	0.68
1350	**Y**	1348	1353	TNYMPY	1.987
1351	**M**	1349	1354	NYMPYF	1.192
1352	**P**	1350	1355	YMPYFF	0.642
1353	**Y**	1351	1356	MPYFFT	0.591
1354	**F**	1352	1357	PYFFTL	0.493
1355	**F**	1353	1358	YFFTLL	0.263
1356	**T**	1354	1359	FFTLLL	0.138
1357	**L**	1355	1360	FTLLLQ	0.277
1358	**L**	1356	1361	TLLLQL	0.263
1359	**L**	1357	1362	LLLQLC	0.098
1360	**Q**	1358	1363	LLQLCT	0.171
1361	**L**	1359	1364	LQLCTF	0.18
1362	**C**	1360	1365	QLCTFT	0.315
1363	**T**	1361	1366	LCTFTR	0.356

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1364	**F**	1362	1367	CTFTRS	0.578
1365	**T**	1363	1368	TFTRST	1.557
1366	**R**	1364	1369	FTRSTN	1.734
1367	**S**	1365	1370	TRSTNS	2.684
1368	**T**	1366	1371	RSTNSR	3.643
1369	**N**	1367	1372	STNSRI	1.304
1370	**S**	1368	1373	TNSRIK	1.946
1371	**R**	1369	1374	NSRIKA	1.362
1372	**I**	1370	1375	SRIKAS	1.135
1373	**K**	1371	1376	RIKASM	0.838
1374	**A**	1372	1377	IKASMP	0.662
1375	**S**	1373	1378	KASMPT	1.362
1376	**M**	1374	1379	ASMPTT	0.983
1377	**P**	1375	1380	SMPTTI	0.682
1378	**T**	1376	1381	MPTTIA	0.514
1379	**T**	1377	1382	PTTIAK	1.039
1380	**I**	1378	1383	TTIAKN	1.081
1381	**A**	1379	1384	TIAKNT	1.081
1382	**K**	1380	1385	IAKNTV	0.556
1383	**N**	1381	1386	AKNTVK	1.586
1384	**T**	1382	1387	KNTVKS	2.103
1385	**V**	1383	1388	NTVKSV	0.781
1386	**K**	1384	1389	TVKSVG	0.48
1387	**S**	1385	1390	VKSVGK	0.666
1388	**V**	1386	1391	KSVGKF	0.777
1389	**G**	1387	1392	SVGKFC	0.208
1390	**K**	1388	1393	VGKFCL	0.128
1391	**F**	1389	1394	GKFCLE	0.299
1392	**C**	1390	1395	KFCLEA	0.305
1393	**L**	1391	1396	FCLEAS	0.204
1394	**E**	1392	1397	CLEASF	0.204
1395	**A**	1393	1398	LEASFN	0.613
1396	**S**	1394	1399	EASFNY	1.166
1397	**F**	1395	1400	ASFNYL	0.555
1398	**N**	1396	1401	SFNYLK	1.099
1399	**Y**	1397	1402	FNYLKS	1.099
1400	**L**	1398	1403	NYLKSP	1.962
1401	**K**	1399	1404	YLKSPN	1.962
1402	**S**	1400	1405	LKSPNF	1.084
1403	**P**	1401	1406	KSPNFS	1.762
1404	**N**	1402	1407	SPNFSK	1.762
1405	**F**	1403	1408	PNFSKL	1.084
1406	**S**	1404	1409	NFSKLI	0.492
1407	**K**	1405	1410	FSKLIN	0.492
1408	**L**	1406	1411	SKLINI	0.398
1409	**I**	1407	1412	KLINII	0.208
1410	**N**	1408	1413	LINIII	0.073

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1411	**I**	1409	1414	INIIIW	0.093
1412	**I**	1410	1415	NIIIWF	0.115
1413	**I**	1411	1416	IIIWFL	0.059
1414	**W**	1412	1417	IIWFLL	0.069
1415	**F**	1413	1418	IWFLLL	0.082
1416	**L**	1414	1419	WFLLLS	0.156
1417	**L**	1415	1420	FLLLSV	0.11
1418	**L**	1416	1421	LLLSVC	0.068
1419	**S**	1417	1422	LLSVCL	0.068
1420	**V**	1418	1423	LSVCLG	0.082
1421	**C**	1419	1424	SVCLGS	0.133
1422	**L**	1420	1425	VCLGSL	0.082
1423	**G**	1421	1426	CLGSLI	0.077
1424	**S**	1422	1427	LGSLIY	0.226
1425	**L**	1423	1428	GSLIYS	0.367
1426	**I**	1424	1429	SLIYST	0.535
1427	**Y**	1425	1430	LIYSTA	0.403
1428	**S**	1426	1431	IYSTAA	0.494
1429	**T**	1427	1432	YSTAAL	0.581
1430	**A**	1428	1433	STAALG	0.367
1431	**A**	1429	1434	TAALGV	0.203
1432	**L**	1430	1435	AALGVL	0.116
1433	**G**	1431	1436	ALGVLM	0.114
1434	**V**	1432	1437	LGVLMS	0.151
1435	**L**	1433	1438	GVLMSN	0.294
1436	**M**	1434	1439	VLMSNL	0.245
1437	**S**	1435	1440	LMSNLG	0.327
1438	**N**	1436	1441	MSNLGM	0.392
1439	**L**	1437	1442	SNLGMP	0.613
1440	**G**	1438	1443	NLGMPS	0.613
1441	**M**	1439	1444	LGMPSY	0.597
1442	**P**	1440	1445	GMPSYC	0.388
1443	**S**	1441	1446	MPSYCT	0.566
1444	**Y**	1442	1447	PSYCTG	0.566
1445	**C**	1443	1448	SYCTGY	0.574
1446	**T**	1444	1449	YCTGYR	0.839
1447	**G**	1445	1450	CTGYRE	0.927
1448	**Y**	1446	1451	TGYREG	1.712
1449	**R**	1447	1452	GYREGY	1.858
1450	**E**	1448	1453	YREGYL	1.549
1451	**G**	1449	1454	REGYLN	1.589
1452	**Y**	1450	1455	EGYLNS	1.087
1453	**L**	1451	1456	GYLNST	0.906
1454	**N**	1452	1457	YLNSTN	1.473
1455	**S**	1453	1458	LNSTNV	0.698
1456	**T**	1454	1459	NSTNVT	1.221
1457	**N**	1455	1460	STNVTI	0.532

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1458	**V**	1456	1461	TNVTIA	0.401
1459	**T**	1457	1462	NVTIAT	0.401
1460	**I**	1458	1463	VTIATY	0.391
1461	**A**	1459	1464	TIATYC	0.282
1462	**T**	1460	1465	IATYCT	0.282
1463	**Y**	1461	1466	ATYCTG	0.398
1464	**C**	1462	1467	TYCTGS	0.529
1465	**T**	1463	1468	YCTGSI	0.257
1466	**G**	1464	1469	CTGSIP	0.253
1467	**S**	1465	1470	TGSIPC	0.253
1468	**I**	1466	1471	GSIPCS	0.235
1469	**P**	1467	1472	SIPCSV	0.176
1470	**C**	1468	1473	IPCSVC	0.071
1471	**S**	1469	1474	PCSVCL	0.083
1472	**V**	1470	1475	CSVCLS	0.072
1473	**C**	1471	1476	SVCLSG	0.133
1474	**L**	1472	1477	VCLSGL	0.082
1475	**S**	1473	1478	CLSGLD	0.184
1476	**G**	1474	1479	LSGLDS	0.46
1477	**L**	1475	1480	SGLDSL	0.46
1478	**D**	1476	1481	GLDSLD	0.573
1479	**S**	1477	1482	LDSLDT	0.836
1480	**L**	1478	1483	DSLDTY	1.588
1481	**D**	1479	1484	SLDTYP	1.47
1482	**T**	1480	1485	LDTYPS	1.47
1483	**Y**	1481	1486	DTYPSL	1.47
1484	**P**	1482	1487	TYPSLE	1.525
1485	**S**	1483	1488	YPSLET	1.525
1486	**L**	1484	1489	PSLETI	0.682
1487	**E**	1485	1490	SLETIQ	0.764
1488	**T**	1486	1491	LETIQI	0.4
1489	**I**	1487	1492	ETIQIT	0.699
1490	**Q**	1488	1493	TIQITI	0.283
1491	**I**	1489	1494	IQITIS	0.263
1492	**T**	1490	1495	QITISS	0.503
1493	**I**	1491	1496	ITISSF	0.251
1494	**S**	1492	1497	TISSFK	0.717
1495	**S**	1493	1498	ISSFKW	0.522
1496	**F**	1494	1499	SSFKWD	1.244
1497	**K**	1495	1500	SFKWDL	0.766
1498	**W**	1496	1501	FKWDLT	0.825
1499	**D**	1497	1502	KWDLTA	0.962
1500	**L**	1498	1503	WDLTAF	0.417
1501	**T**	1499	1504	DLTAFG	0.392
1502	**A**	1500	1505	LTAFGL	0.194
1503	**F**	1501	1506	TAFGLV	0.174
1504	**G**	1502	1507	AFGLVA	0.122

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1505	**L**	1503	1508	FGLVAE	0.209
1506	**V**	1504	1509	GLVAEW	0.254
1507	**A**	1505	1510	LVAEWF	0.222
1508	**E**	1506	1511	VAEWFL	0.222
1509	**W**	1507	1512	AEWFLA	0.302
1510	**F**	1508	1513	EWFLAY	0.469
1511	**L**	1509	1514	WFLAYI	0.19
1512	**A**	1510	1515	FLAYIL	0.149
1513	**Y**	1511	1516	LAYILF	0.149
1514	**I**	1512	1517	AYILFT	0.261
1515	**L**	1513	1518	YILFTR	0.505
1516	**F**	1514	1519	ILFTRF	0.279
1517	**T**	1515	1520	LFTRFF	0.345
1518	**R**	1516	1521	FTRFFY	0.655
1519	**F**	1517	1522	TRFFYV	0.562
1520	**F**	1518	1523	RFFYVL	0.321
1521	**Y**	1519	1524	FFYVLG	0.162
1522	**V**	1520	1525	FYVLGL	0.154
1523	**L**	1521	1526	YVLGLA	0.18
1524	**G**	1522	1527	VLGLAA	0.116
1525	**L**	1523	1528	LGLAAI	0.11
1526	**A**	1524	1529	GLAAIM	0.132
1527	**A**	1525	1530	LAAIMQ	0.23
1528	**I**	1526	1531	AAIMQL	0.23
1529	**M**	1527	1532	AIMQLF	0.197
1530	**Q**	1528	1533	IMQLFF	0.169
1531	**L**	1529	1534	MQLFFS	0.324
1532	**F**	1530	1535	QLFFSY	0.512
1533	**F**	1531	1536	LFFSYF	0.256
1534	**S**	1532	1537	FFSYFA	0.314
1535	**Y**	1533	1538	FSYFAV	0.269
1536	**F**	1534	1539	SYFAVH	0.423
1537	**A**	1535	1540	YFAVHF	0.273
1538	**V**	1536	1541	FAVHFI	0.122
1539	**H**	1537	1542	AVHFIS	0.189
1540	**F**	1538	1543	VHFISN	0.301
1541	**I**	1539	1544	HFISNS	0.543
1542	**S**	1540	1545	FISNSW	0.42
1543	**N**	1541	1546	ISNSWL	0.4
1544	**S**	1542	1547	SNSWLM	0.565
1545	**W**	1543	1548	NSWLMW	0.443
1546	**L**	1544	1549	SWLMWL	0.227
1547	**M**	1545	1550	WLMWLI	0.119
1548	**W**	1546	1551	LMWLII	0.079
1549	**L**	1547	1552	MWLIIN	0.154
1550	**I**	1548	1553	WLIINL	0.129
1551	**I**	1549	1554	LIINLV	0.091

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1552	**N**	1550	1555	IINLVQ	0.191
1553	**L**	1551	1556	INLVQM	0.269
1554	**V**	1552	1557	NLVQMA	0.388
1555	**Q**	1553	1558	LVQMAP	0.373
1556	**M**	1554	1559	VQMAPI	0.317
1557	**A**	1555	1560	QMAPIS	0.573
1558	**P**	1556	1561	MAPISA	0.334
1559	**I**	1557	1562	APISAM	0.334
1560	**S**	1558	1563	PISAMV	0.246
1561	**A**	1559	1564	ISAMVR	0.311
1562	**M**	1560	1565	SAMVRM	0.439
1563	**V**	1561	1566	AMVRMY	0.513
1564	**R**	1562	1567	MVRMYI	0.356
1565	**M**	1563	1568	VRMYIF	0.312
1566	**Y**	1564	1569	RMYIFF	0.364
1567	**I**	1565	1570	MYIFFA	0.188
1568	**F**	1566	1571	YIFFAS	0.254
1569	**F**	1567	1572	IFFASF	0.14
1570	**A**	1568	1573	FFASFY	0.314
1571	**S**	1569	1574	FASFYY	0.568
1572	**F**	1570	1575	ASFYYV	0.487
1573	**Y**	1571	1576	SFYYVW	0.507
1574	**Y**	1572	1577	FYYVWK	0.756
1575	**V**	1573	1578	YYVWKS	1.17
1576	**W**	1574	1579	YVWKSY	1.17
1577	**K**	1575	1580	VWKSYV	0.554
1578	**S**	1576	1581	WKSYVH	1.016
1579	**Y**	1577	1582	KSYVHV	0.717
1580	**V**	1578	1583	SYVHVV	0.266
1581	**H**	1579	1584	YVHVVD	0.332
1582	**V**	1580	1585	VHVVDG	0.209
1583	**V**	1581	1586	HVVDGC	0.151
1584	**D**	1582	1587	VVDGCN	0.179
1585	**G**	1583	1588	VDGCNS	0.323
1586	**C**	1584	1589	DGCNSS	0.583
1587	**N**	1585	1590	GCNSST	0.504
1588	**S**	1586	1591	CNSSTC	0.273
1589	**S**	1587	1592	NSSTCM	0.504
1590	**T**	1588	1593	SSTCMM	0.31
1591	**C**	1589	1594	STCMMC	0.124
1592	**M**	1590	1595	TCMMCY	0.145
1593	**M**	1591	1596	CMMCYK	0.201
1594	**C**	1592	1597	MMCYKR	0.734
1595	**Y**	1593	1598	MCYKRN	1.193
1596	**K**	1594	1599	CYKRNR	2.361
1597	**R**	1595	1600	YKRNRA	4.449
1598	**N**	1596	1601	KRNRAT	4.098

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1599	**R**	1597	1602	RNRATR	4.014
1600	**A**	1598	1603	NRATRV	1.521
1601	**T**	1599	1604	RATRVE	1.638
1602	**R**	1600	1605	ATRVEC	0.448
1603	**V**	1601	1606	TRVECT	0.64
1604	**E**	1602	1607	RVECTT	0.64
1605	**C**	1603	1608	VECTTI	0.229
1606	**T**	1604	1609	ECTTIV	0.229
1607	**T**	1605	1610	CTTIVN	0.213
1608	**I**	1606	1611	TTIVNG	0.393
1609	**V**	1607	1612	TIVNGV	0.202
1610	**N**	1608	1613	IVNGVR	0.274
1611	**G**	1609	1614	VNGVRR	0.766
1612	**V**	1610	1615	NGVRRS	1.384
1613	**R**	1611	1616	GVRRSF	0.745
1614	**R**	1612	1617	VRRSFY	1.18
1615	**S**	1613	1618	RRSFYV	1.18
1616	**F**	1614	1619	RSFYVY	0.944
1617	**Y**	1615	1620	SFYVYA	0.487
1618	**V**	1616	1621	FYVYAN	0.584
1619	**Y**	1617	1622	YVYANG	0.667
1620	**A**	1618	1623	VYANGG	0.422
1621	**N**	1619	1624	YANGGK	1.136
1622	**G**	1620	1625	ANGGKG	0.717
1623	**G**	1621	1626	NGGKGF	0.615
1624	**K**	1622	1627	GGKGFC	0.205
1625	**G**	1623	1628	GKGFCK	0.414
1626	**F**	1624	1629	KGFCKL	0.345
1627	**C**	1625	1630	GFCKLH	0.235
1628	**K**	1626	1631	FCKLHN	0.382
1629	**L**	1627	1632	CKLHNW	0.463
1630	**H**	1628	1633	KLHNWN	1.39
1631	**N**	1629	1634	LHNWNC	0.373
1632	**W**	1630	1635	HNWNCV	0.335
1633	**N**	1631	1636	NWNCVN	0.396
1634	**C**	1632	1637	WNCVNC	0.132
1635	**V**	1633	1638	NCVNCD	0.21
1636	**N**	1634	1639	CVNCDT	0.188
1637	**C**	1635	1640	VNCDTF	0.304
1638	**D**	1636	1641	NCDTFC	0.22
1639	**T**	1637	1642	CDTFCA	0.138
1640	**F**	1638	1643	DTFCAG	0.255
1641	**C**	1639	1644	TFCAGS	0.204
1642	**A**	1640	1645	FCAGST	0.204
1643	**G**	1641	1646	CAGSTF	0.204
1644	**S**	1642	1647	AGSTFI	0.267
1645	**T**	1643	1648	GSTFIS	0.355

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1646	**F**	1644	1649	STFISD	0.599
1647	**I**	1645	1650	TFISDE	0.774
1648	**S**	1646	1651	FISDEV	0.398
1649	**D**	1647	1652	ISDEVA	0.464
1650	**E**	1648	1653	SDEVAR	1.297
1651	**V**	1649	1654	DEVARD	1.616
1652	**A**	1650	1655	EVARDL	0.798
1653	**R**	1651	1656	VARDLS	0.618
1654	**D**	1652	1657	ARDLSL	0.686
1655	**L**	1653	1658	RDLSLQ	1.176
1656	**S**	1654	1659	DLSLQF	0.52
1657	**L**	1655	1660	LSLQFK	0.623
1658	**Q**	1656	1661	SLQFKR	1.479
1659	**F**	1657	1662	LQFKRP	1.707
1660	**K**	1658	1663	QFKRPI	1.451
1661	**R**	1659	1664	FKRPIN	1.347
1662	**P**	1660	1665	KRPINP	2.405
1663	**I**	1661	1666	RPINPT	1.736
1664	**N**	1662	1667	PINPTD	1.48
1665	**P**	1663	1668	INPTDQ	1.658
1666	**T**	1664	1669	NPTDQS	3.169
1667	**D**	1665	1670	PTDQSS	2.641
1668	**Q**	1666	1671	TDQSSY	2.676
1669	**S**	1667	1672	DQSSYI	1.3
1670	**S**	1668	1673	QSSYIV	0.578
1671	**Y**	1669	1674	SSYIVD	0.557
1672	**I**	1670	1675	SYIVDS	0.557
1673	**V**	1671	1676	YIVDSV	0.309
1674	**D**	1672	1677	IVDSVT	0.284
1675	**S**	1673	1678	VDSVTV	0.301
1676	**V**	1674	1679	DSVTVK	0.811
1677	**T**	1675	1680	SVTVKN	0.781
1678	**V**	1676	1681	VTVKNG	0.576
1679	**K**	1677	1682	TVKNGS	1.041
1680	**N**	1678	1683	VKNGSI	0.506
1681	**G**	1679	1684	KNGSIH	0.927
1682	**S**	1680	1685	NGSIHL	0.382
1683	**I**	1681	1686	GSIHLY	0.372
1684	**H**	1682	1687	SIHLYF	0.326
1685	**L**	1683	1688	IHLYFD	0.406
1686	**Y**	1684	1689	HLYFDK	1.159
1687	**F**	1685	1690	LYFDKA	0.86
1688	**D**	1686	1691	YFDKAG	1.032
1689	**K**	1687	1692	FDKAGQ	1.141
1690	**A**	1688	1693	DKAGQK	2.635
1691	**G**	1689	1694	KAGQKT	2.277
1692	**Q**	1690	1695	AGQKTY	1.784

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1693	**K**	1691	1696	GQKTYE	3.058
1694	**T**	1692	1697	QKTYER	6.053
1695	**Y**	1693	1698	KTYERH	4.756
1696	**E**	1694	1699	TYERHS	3.187
1697	**R**	1695	1700	YERHSL	1.821
1698	**H**	1696	1701	ERHSLS	1.557
1699	**S**	1697	1702	RHSLSH	1.224
1700	**L**	1698	1703	HSLSHF	0.541
1701	**S**	1699	1704	SLSHFV	0.295
1702	**H**	1700	1705	LSHFVN	0.354
1703	**F**	1701	1706	SHFVNL	0.354
1704	**V**	1702	1707	HFVNLD	0.441
1705	**N**	1703	1708	FVNLDN	0.522
1706	**L**	1704	1709	VNLDNL	0.497
1707	**D**	1705	1710	NLDNLR	1.311
1708	**N**	1706	1711	LDNLRA	0.823
1709	**L**	1707	1712	DNLRAN	1.606
1710	**R**	1708	1713	NLRANN	1.546
1711	**A**	1709	1714	LRANNT	1.388
1712	**N**	1710	1715	RANNTK	3.365
1713	**N**	1711	1716	ANNTKG	1.7
1714	**T**	1712	1717	NNTKGS	2.255
1715	**K**	1713	1718	NTKGSL	1.157
1716	**G**	1714	1719	TKGSLP	1.112
1717	**S**	1715	1720	KGSLPI	0.54
1718	**L**	1716	1721	GSLPIN	0.434
1719	**P**	1717	1722	SLPINV	0.326
1720	**I**	1718	1723	LPINVI	0.17
1721	**N**	1719	1724	PINVIV	0.153
1722	**V**	1720	1725	INVIVF	0.086
1723	**I**	1721	1726	NVIVFD	0.205
1724	**V**	1722	1727	VIVFDG	0.126
1725	**F**	1723	1728	IVFDGK	0.339
1726	**D**	1724	1729	VFDGKS	0.649
1727	**G**	1725	1730	FDGKSK	1.747
1728	**K**	1726	1731	DGKSKC	1.082
1729	**S**	1727	1732	GKSKCE	1.122
1730	**K**	1728	1733	KSKCEE	1.963
1731	**C**	1729	1734	SKCEES	1.316
1732	**E**	1730	1735	KCEESS	1.316
1733	**E**	1731	1736	CEESSA	0.665
1734	**S**	1732	1737	EESSAK	2.479
1735	**S**	1733	1738	ESSAKS	1.919
1736	**A**	1734	1739	SSAKSA	1.119
1737	**K**	1735	1740	SAKSAS	1.119
1738	**S**	1736	1741	AKSASV	0.62
1739	**A**	1737	1742	KSASVY	0.961

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1740	**S**	1738	1743	SASVYY	0.753
1741	**V**	1739	1744	ASVYYS	0.753
1742	**Y**	1740	1745	SVYYSQ	1.291
1743	**Y**	1741	1746	VYYSQL	0.795
1744	**S**	1742	1747	YYSQLM	1.06
1745	**Q**	1743	1748	YSQLMC	0.362
1746	**L**	1744	1749	SQLMCQ	0.401
1747	**M**	1745	1750	QLMCQP	0.462
1748	**C**	1746	1751	LMCQPI	0.187
1749	**Q**	1747	1752	MCQPIL	0.187
1750	**P**	1748	1753	CQPILL	0.156
1751	**I**	1749	1754	QPILLL	0.24
1752	**L**	1750	1755	PILLLD	0.231
1753	**L**	1751	1756	ILLLDQ	0.259
1754	**L**	1752	1757	LLLDQA	0.373
1755	**D**	1753	1758	LLDQAL	0.373
1756	**Q**	1754	1759	LDQALV	0.336
1757	**A**	1755	1760	DQALVS	0.546
1758	**L**	1756	1761	QALVSD	0.546
1759	**V**	1757	1762	ALVSDV	0.234
1760	**S**	1758	1763	LVSDVG	0.229
1761	**D**	1759	1764	VSDVGD	0.464
1762	**V**	1760	1765	SDVGDS	0.838
1763	**G**	1761	1766	DVGDSA	0.632
1764	**D**	1762	1767	VGDSAE	0.655
1765	**S**	1763	1768	GDSAEV	0.655
1766	**A**	1764	1769	DSAEVA	0.669
1767	**E**	1765	1770	SAEVAV	0.297
1768	**V**	1766	1771	AEVAVK	0.444
1769	**A**	1767	1772	EVAVKM	0.435
1770	**V**	1768	1773	VAVKMF	0.217
1771	**K**	1769	1774	AVKMFD	0.489
1772	**M**	1770	1775	VKMFDA	0.489
1773	**F**	1771	1776	KMFDAY	1.032
1774	**D**	1772	1777	MFDAYV	0.383
1775	**A**	1773	1778	FDAYVN	0.622
1776	**Y**	1774	1779	DAYVNT	1.037
1777	**V**	1775	1780	AYVNTF	0.538
1778	**N**	1776	1781	YVNTFS	0.714
1779	**T**	1777	1782	VNTFSS	0.61
1780	**F**	1778	1783	NTFSST	1.187
1781	**S**	1779	1784	TFSSTF	0.639
1782	**S**	1780	1785	FSSTFN	0.712
1783	**T**	1781	1786	SSTFNV	0.61
1784	**F**	1782	1787	STFNVP	0.704
1785	**N**	1783	1788	TFNVPM	0.52
1786	**V**	1784	1789	FNVPME	0.624

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1787	**P**	1785	1790	NVPMEK	1.441
1788	**M**	1786	1791	VPMEKL	0.739
1789	**E**	1787	1792	PMEKLK	1.991
1790	**K**	1788	1793	MEKLKT	1.859
1791	**L**	1789	1794	EKLKTL	1.549
1792	**K**	1790	1795	KLKTLV	0.664
1793	**T**	1791	1796	LKTLVA	0.335
1794	**L**	1792	1797	KTLVAT	0.587
1795	**V**	1793	1798	TLVATA	0.296
1796	**A**	1794	1799	LVATAE	0.356
1797	**T**	1795	1800	VATAEA	0.436
1798	**A**	1796	1801	ATAEAE	1.017
1799	**E**	1797	1802	TAEAEL	0.83
1800	**A**	1798	1803	AEAELA	0.581
1801	**E**	1799	1804	EAELAK	1.15
1802	**L**	1800	1805	AELAKN	1.068
1803	**A**	1801	1806	ELAKNV	0.785
1804	**K**	1802	1807	LAKNVS	0.607
1805	**N**	1803	1808	AKNVSL	0.607
1806	**V**	1804	1809	KNVSLD	1.004
1807	**S**	1805	1810	NVSLDN	0.807
1808	**L**	1806	1811	VSLDNV	0.373
1809	**D**	1807	1812	SLDNVL	0.414
1810	**N**	1808	1813	LDNVLS	0.414
1811	**V**	1809	1814	DNVLST	0.724
1812	**L**	1810	1815	NVLSTF	0.376
1813	**S**	1811	1816	VLSTFI	0.164
1814	**T**	1812	1817	LSTFIS	0.296
1815	**F**	1813	1818	STFISA	0.362
1816	**I**	1814	1819	TFISAA	0.273
1817	**S**	1815	1820	FISAAR	0.37
1818	**A**	1816	1821	ISAARQ	0.741
1819	**A**	1817	1822	SAARQG	1.046
1820	**R**	1818	1823	AARQGF	0.676
1821	**Q**	1819	1824	ARQGFV	0.497
1822	**G**	1820	1825	RQGFVD	0.821
1823	**F**	1821	1826	QGFVDS	0.562
1824	**V**	1822	1827	GFVDSD	0.542
1825	**D**	1823	1828	FVDSDV	0.406
1826	**S**	1824	1829	VDSDVE	0.812
1827	**D**	1825	1830	DSDVET	1.58
1828	**V**	1826	1831	SDVETK	1.892
1829	**E**	1827	1832	DVETKD	2.357
1830	**T**	1828	1833	VETKDV	1.048
1831	**K**	1829	1834	ETKDVV	1.048
1832	**D**	1830	1835	TKDVVE	1.048
1833	**V**	1831	1836	KDVVEC	0.389
1834	**V**	1832	1837	DVVECL	0.16

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1835	**E**	1833	1838	VVECLK	0.192
1836	**C**	1834	1839	VECLKL	0.214
1837	**L**	1835	1840	ECLKLS	0.386
1838	**K**	1836	1841	CLKLSH	0.303
1839	**L**	1837	1842	LKLSHQ	0.979
1840	**S**	1838	1843	KLSHQS	1.59
1841	**H**	1839	1844	LSHQSD	1.328
1842	**Q**	1840	1845	SHQSDI	1.129
1843	**S**	1841	1846	HQSDIE	1.459
1844	**D**	1842	1847	QSDIEV	0.796
1845	**I**	1843	1848	SDIEVT	0.663
1846	**E**	1844	1849	DIEVTG	0.49
1847	**V**	1845	1850	IEVTGD	0.49
1848	**T**	1846	1851	EVTGDS	0.936
1849	**G**	1847	1852	VTGDSC	0.29
1850	**D**	1848	1853	TGDSCN	0.628
1851	**S**	1849	1854	GDSCNN	0.699
1852	**C**	1850	1855	DSCNNY	1.108
1853	**N**	1851	1856	SCNNYM	0.656
1854	**N**	1852	1857	CNNYML	0.404
1855	**Y**	1853	1858	NNYMLT	1.087
1856	**M**	1854	1859	NYMLTY	1.06
1857	**L**	1855	1860	YMLTYN	1.06
1858	**T**	1856	1861	MLTYNK	1.352
1859	**Y**	1857	1862	LTYNKV	1.014
1860	**N**	1858	1863	TYNKVE	2.13
1861	**K**	1859	1864	YNKVEN	2.373
1862	**V**	1860	1865	NKVENM	1.499
1863	**E**	1861	1866	KVENMT	1.345
1864	**N**	1862	1867	VENMTP	1.04
1865	**M**	1863	1868	ENMTPR	2.745
1866	**T**	1864	1869	NMTPRD	2.647
1867	**P**	1865	1870	MTPRDL	1.357
1868	**R**	1866	1871	TPRDLG	1.357
1869	**D**	1867	1872	PRDLGA	0.95
1870	**L**	1868	1873	RDLGAC	0.329
1871	**G**	1869	1874	DLGACI	0.118
1872	**A**	1870	1875	LGACID	0.118
1873	**C**	1871	1876	GACIDC	0.077
1874	**I**	1872	1877	ACIDCS	0.104
1875	**D**	1873	1878	CIDCSA	0.104
1876	**C**	1874	1879	IDCSAR	0.379
1877	**S**	1875	1880	DCSARH	0.736
1878	**A**	1876	1881	CSARHI	0.309
1879	**R**	1877	1882	SARHIN	0.927
1880	**H**	1878	1883	ARHINA	0.699
1881	**I**	1879	1884	RHINAQ	1.198
1882	**N**	1880	1885	HINAQV	0.454

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1883	**A**	1881	1886	INAQVA	0.337
1884	**Q**	1882	1887	NAQVAK	0.961
1885	**V**	1883	1888	AQVAKS	0.801
1886	**A**	1884	1889	QVAKSH	1.079
1887	**K**	1885	1890	VAKSHN	1.002
1888	**S**	1886	1891	AKSHNI	0.946
1889	**H**	1887	1892	KSHNIA	0.946
1890	**N**	1888	1893	SHNIAL	0.39
1891	**I**	1889	1894	HNIALI	0.204
1892	**A**	1890	1895	NIALIW	0.158
1893	**L**	1891	1896	IALIWN	0.158
1894	**I**	1892	1897	ALIWNV	0.167
1895	**W**	1893	1898	LIWNVK	0.331
1896	**N**	1894	1899	IWNVKD	0.669
1897	**V**	1895	1900	WNVKDF	0.827
1898	**K**	1896	1901	NVKDFM	0.778
1899	**D**	1897	1902	VKDFMS	0.649
1900	**F**	1898	1903	KDFMSL	0.721
1901	**M**	1899	1904	DFMSLS	0.483
1902	**S**	1900	1905	FMSLSE	0.501
1903	**L**	1901	1906	MSLSEQ	1.002
1904	**S**	1902	1907	SLSEQL	0.835
1905	**E**	1903	1908	LSEQLR	1.22
1906	**Q**	1904	1909	SEQLRK	2.958
1907	**L**	1905	1910	EQLRKQ	3.823
1908	**R**	1906	1911	QLRKQI	1.547
1909	**K**	1907	1912	LRKQIR	1.75
1910	**Q**	1908	1913	RKQIRS	2.844
1911	**I**	1909	1914	KQIRSA	1.467
1912	**R**	1910	1915	QIRSAA	0.741
1913	**S**	1911	1916	IRSAAK	0.856
1914	**A**	1912	1917	RSAAKK	2.441
1915	**A**	1913	1918	SAAKKN	2.004
1916	**K**	1914	1919	AAKKNN	2.405
1917	**K**	1915	1920	AKKNNL	1.963
1918	**N**	1916	1921	KKNNLP	3.005
1919	**N**	1917	1922	KNNLPF	1.301
1920	**L**	1918	1923	NNLPFK	1.301
1921	**P**	1919	1924	NLPFKL	0.667
1922	**F**	1920	1925	LPFKLT	0.599
1923	**K**	1921	1926	PFKLTC	0.389
1924	**L**	1922	1927	FKLTCA	0.254
1925	**T**	1923	1928	KLTCAT	0.424
1926	**C**	1924	1929	LTCATT	0.306
1927	**A**	1925	1930	TCATTR	0.726
1928	**T**	1926	1931	CATTRQ	0.872
1929	**T**	1927	1932	ATTRQV	1.207
1930	**R**	1928	1933	TTRQVV	0.887

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1931	**Q**	1929	1934	TRQVVN	0.988
1932	**V**	1930	1935	RQVVNV	0.508
1933	**V**	1931	1936	QVVNVV	0.193
1934	**N**	1932	1937	VVNVVT	0.16
1935	**V**	1933	1938	VNVVTT	0.312
1936	**V**	1934	1939	NVVTTK	0.841
1937	**T**	1935	1940	VVTTKI	0.366
1938	**T**	1936	1941	VTTKIA	0.499
1939	**K**	1937	1942	TTKIAL	0.554
1940	**I**	1938	1943	TKIALK	0.768
1941	**A**	1939	1944	KIALKG	0.527
1942	**L**	1940	1945	IALKGG	0.261

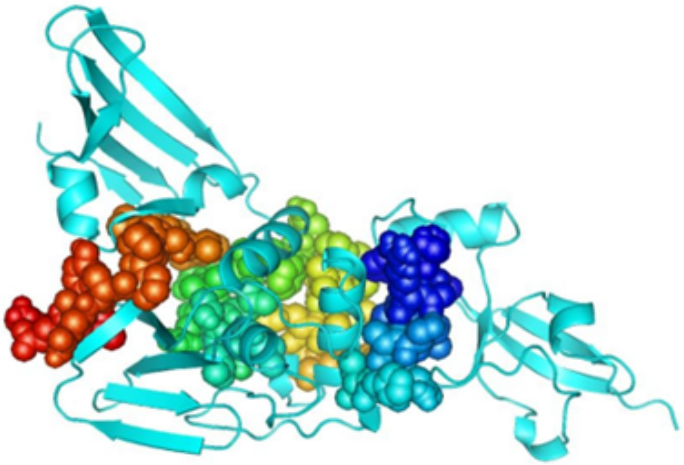

Figure 2: Specific sites of B cells predicted linear epitopes on the 3D structure of PLpro Protein

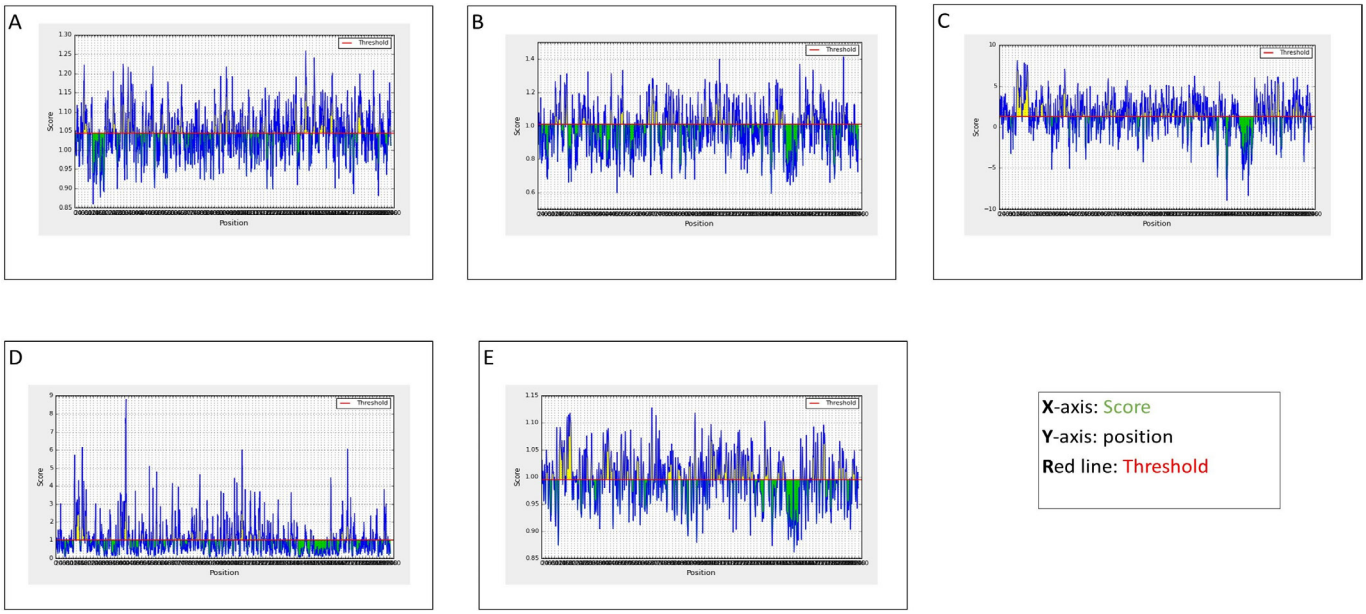

Figure 3: (A) Prediction of antigenic determinants of PLpro protein using Kolaskar and Tongaonkar Antigenicity Scale; (B) Beta turns analyses in PLpro protein using Chou and Fasman Beta Turn Prediction; (C) Hydrophilicity Prediction of using PLpro protein Parker Hydrophilicity; (D) Surface Accessibility Analyses of PLpro protein using Emini Surface Accessibility Scale; (E) Flexibility Analyses of PLpro protein using Karplus and Schulz Flexibility Scale.

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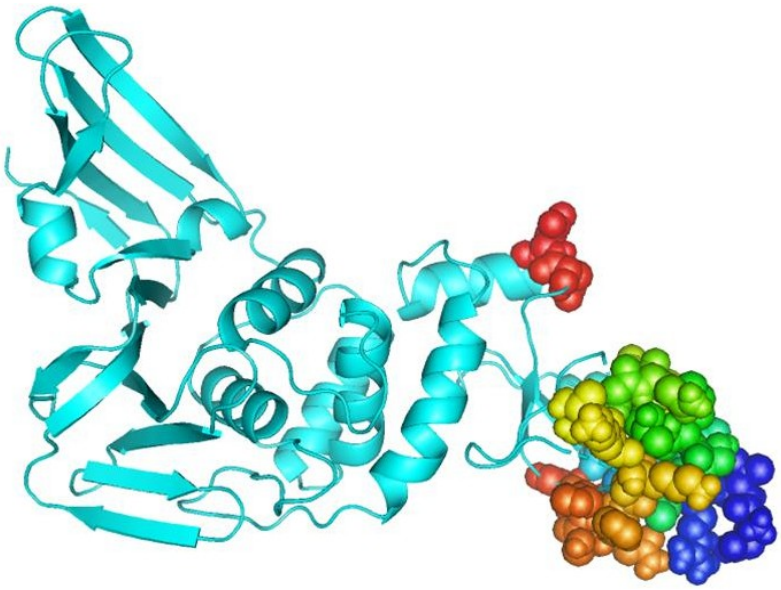

Figure 4: Specific sites of B cells discontinuous epitopes predicted through DISCOTOPE 2.0 server on the 3D structure of PLpro protein

Table 2: Discontinuous epitopes predicted through DiscoTop 2.0 server

Residues Position	Residues Name	Number of Contacts	Propensity Score	Discotop Score
746	GLU	4	2.165	1.456
747	VAL	3	1.617	1.086
748	ARG	12	1.266	-0.26
749	THR	8	0.303	-0.652
750	ILE	19	-0.128	-2.378
751	LYS	3	-0.5	-0.788
763	THR	3	-3.163	-3.144
765	VAL	3	-0.715	-0.977
767	ASP	10	0.338	-0.85
768	MET	12	1.024	-0.474
769	SER	3	1.2	0.717
770	MET	9	1.122	-0.042
771	THR	13	0.48	-1.07
773	GLY	10	-0.637	-1.714
774	GLN	11	0.154	-1.129
775	GLN	26	-0.562	-3.487
787	THR	10	-1.994	-2.915
788	LYS	2	-0.051	-0.275
789	ILE	11	0.306	-0.994
790	LYS	8	0.659	-0.337
791	PRO	28	0.942	-2.386
792	HIS	10	1.274	-0.023
793	ASN	3	1.662	1.126
794	SER	5	1.496	0.749
795	HIS	29	0.839	-2.539
796	GLU	5	-0.023	-0.059
797	GLY	1	-0.103	-1.012
806	ASP	8	-2.763	-3.366
807	ASP	0	-2.535	-2.244

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T cell epitopes prediction and properties evaluation

IEDB consensus method was used to forecast T-cell MHC Class-I as well as MHC class-II epitopes. Peptides due to strong defensive ability can be bind to multiple alleles therefore; this peptide is considered most appropriate. Their Allergenicity and Antigenicity were checked by Allergen FP 1.0 and VaxiJen respectively and IEDB conservancy tool was used for their conservation analysis of protein sequence. Epitopes that are 100% conserved, highly antigenic, non-allergenicand bound to multiple alleles were screened out. 6 MHC-class-I and 6 MHC class- II alleles were shortlisted. Between MHC class-I epitopes 'YHTTDPSFLGRY' has the highest antigenicity (1.3) binding with multiple alleles including HLA-A*01:01HLA-A*26:01, HLA- A*29:02, HLA-A*30:02, HLA-A*25:01, HLA-B*38:01, HLA-A*68:01(Table 3). In MHC class-II epitopes 'PFVMMSAPPAQYELK' had higher Antigenicity score(0.8) binding with multiple alleles HLA-DRB1*01:02, HLA-DRB1*09:01, HLA-DRB1*01:01, HLA-DRB1*13:07, HLA-DRB1*04:08, HLA-DRB1*11:07, HLA-DRB1*11:14, HLA-DRB1*13:23, HLA-DRB1*03:05 (Table 4). To estimate peptide digesting enzymes, the protein digesting enzyme server was used. The enzymes that do not digest peptide into fragments is considered a non- digestive enzyme. Peptides that are digestible with multiple enzymes are not stable. Peptides that are digested with fewer enzymes are considered most stable and favorable for vaccine (Table 5).

Population coverage of Peptides

Population coverage was foundforthe selectedsix MHC class-I and six MHC class-II epitopes and related alleles. Epitopes that were selected represent 94.70% and 44.02% of total world population respectively. Highest population coverage of MHC class-I epitopes was found in Germany (97.14 %) and MHC class -II epitopes was found in Sweden (67.80%).SARS-COV-2 MHC class -I epitopes displayed 91.28 % and MHC class -II exhibited 28.71% population coverage in China. Population coverage was higher in those regions where SARS-COV-2 cases were reported (Figure 5).

Molecular Docking

3D structures of selected six MHC class I epitopes were forecasted using PEPFOLD (Figure 6). Molecular docking is necessary to understand the pattern of interaction between protein and peptide. By performing molecular docking the interaction of HLA allele with selected MHC class I epitope was analyzed. To analyze the interaction between allele and peptides, ClusPro (v.2) webserver was used. Rigid docking was performed by the server by sampling billions of conformations, energy minimization and RMSD of the complex [47]. Pymol was used to visualize the docked complexes. Docking results revealed the strong interactions among all selected peptides inside the receptor binding site of HLA allele (Figure 7).

Table 3: MHC class I binding peptides with their antigenicity score

Peptide(position)	Alleles	Antigenicity
	MHC Class 1	
YHTTDPSFLGRY(25-36)	HLA-A*01:01, HLA-A*26:01,HLA-A*29:02 HLA-A*30:02, HLA-A*25:01, HLA-B*38:01 HLA-A*68:01	1.3
ETISLAGSYKDW (33-44)	HLA-A*25:01, HLA-A*26:01, HLA-B*57:01 HLA-B*58:01, HLA-A*68:01	0.8
FGLVAEWFLAYI(11-22)	HLA-A*26:01, HLA-A*25:01, HLA-A*29:02 HLA-B*35:01, HLA-A*01:01, HLA-C*08:02 HLA-A*02:01, HLA-B*46:01, HLA-B*15:02 HLA-A*68:02 , HLA-C*12:03	0.5
GVVDYGARFYFY(14-25)	HLA-A*29:02, HLA-A*01:01, HLA-C*05:01 HLA-A*30:02, HLA-A*26:01, HLA-A*11:01 HLA-A*23:01	0.7
DLTAFGLVAEWF(7-18)	HLA-B*46:01, HLA-B*57:01	0.6
YYSQLMCQPILL(40-51)	HLA-A*02:01, HLA-A*24:02, HLA-C*14:02 HLA-C*07:02, HLA-B*48:01, HLA-A*23:01 HLA-B*38:01	

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Table 4: MHC class II binding peptides with their antigenicity score

Peptide(position)	Alleles	Antigenicity
-	**MHC Class 2**	
SPFVMMSAPPAQYEL(52-66)	HLA-DRB1*01:01,HLA DRB1*01:02,HLA-DRB1*09:01, HLA-DRB1*13:07,HLA DRB1*04:08,HLA-DRB1*11:07,HLA- DRB1*11:14,HLA-DRB1*13:23, HLA-DRB1*03:05HLA-DRB1*04:04,HLA-DRB1*08:02	0.5
KSAFYILPSIISNEK(20-34)	HLA-DRB1*04:08, HLA-DRB1*04:26, HLA-DRB1*01:01,HLA-DRB1*11:01, HLA-DRB1*04:21, HLA-DRB1*11:28,HLA-DRB1*13:05, HLA-DRB1*13:07,HLA-DRB1*04:01,HLA-DRB1*13:21	0.7
SAFYILPSIISNEKQ(21-35)	D R B 1 * 1 3 : 0 7 , H L A - D R B 1 * 0 4 : 0 1 , H L A - D R B 1 * 1 3 : 2 1 HLA-DRB1*04:08,HLA-DRB1*04:26, HLA-DRB1*11:01,HLA-DRB1*04:21, HLA-DRB1*11:28, HLA-DRB1*13:05,HLA-DRB1*01:01, HLA- DRB1*13:07, HLA-DRB1*04:01,HLA-DRB1*13:21	0.6
EVITFDNLKTLLSLR(9-23)	HLA-DRB1*04:01, HLA-DRB1*15:06, HLA-DRB1*04:04	0.5
PFVMMSAPPAQYELK(53-67)	HLA-DRB1*01:02, HLA-DRB1*09:01, HLA-DRB1*01:01,HLA-DRB1*13:07, HLA-DRB1*04:08, HLA-DRB1*11:07,HLA-DRB1*11:14, HLA- DRB1*13:23, HLA-DRB1*03:05,HLA-DRB1*08:02	0.8
QQESPFVMMSAPPAQ(49-63)	HLA-DRB1*01:02, HLA-DRB1*01:01, HLA-DRB1*09:01,HLA-DRB1*13:07, HLA-DRB1*04:08, HLA-DRB1*11:07,HLA-DRB1*11:14, HLA-DRB1*13:23,HLA-DRB1*03:05,HLA-DRB1*08:02	0.6

Table 5: Peptides that are digested with fewer enzymes are considered most stable and favorable for vaccine.

Peptides	Non-Digesting Enzyme	Allergenicity	Hydrophilicity	Toxicity	Hydrophobicity	Charge	pI	M.W
				MHC Class I				
YHTTDPSFLGRY	Cyanogen_Bromide, IodosoBenzoate, Staph_ ProteaseTr ypsin_K	NA	NT	-0.32	-0.19	0.5	6.74	1456.74
ETISLAGSYKDW	Clostripain Cyanogen_Bromide, IodosoBenzoate Proline_Endopept Staph_Protease Trypsin_R Staph_Protease Trypsin_R	NA	NT	0.05	-0.09	-1.00	4.37	1369.66
FGLVAEWFLAYI	Trypsin, Clostripain ,Cyanogen_Bromide	NA	NT	-1.3	0.33	-1.00	4.00	1428.87
GVVDYGARFYFY	Cyanogen_Bromide ,IodosoBenzoate Staph_Protease, Trypsin_K	NA	NT	-0.78	0.04	0.00	5.83	1456.78
DLTAFGLVAEWF	Trypsin, Clostripain, Cyanogen_Bromide, Proline_Endopept, Trypsin_K Trypsin_R , AspN	NA	NT	-0.74	0.19	-2.00	3.67	1368.72

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YYSQLMCQPILL	Trypsin Clostripain IodosoBenzoate Staph_Protease Trypsin_K Trypsin_R AspN	NA	NT	-1.12	0.08	0.00	5.52	1471.98
				MHC Class II				
SPFVMMSAPPAQYEL	Trypsin, Clostripain, IodosoBenzoate Trypsin_K, Trypsin_R, AspN	NA	NT	-0.53	0.05	-1.00	4.00	1668.16
KSAFYILPSIISNEK	Clostripain, Cyanogen_Bromide, IodosoBenzoate, Trypsin_R, AspN	NA	NT	-0.16	-0.05	1.00	8.50	1710.22
SAFYILPSIISNEKQ	Clostripain Cyanogen_Bromide, IodosoBenzoate, Trypsin_R, AspN Cyanogen_Bromide, IodosoBenzoate, Trypsin_R, AspN	NA	NT	-0.35	-0.02	0.00	5.72	1710.18
EVITFDNLKTLLSLR	Clostripain Cyanogen_Bromide IodosoBenzoate Proline_Endopept Trypsin_R	NA	NT	-0.09	-0.1	0.00	6.17	1762.31
PFVMMSAPPAQYELK	Trypsin, Clostripain IodosoBenzoate Trypsin_K, Trypsin_R,AspN	NA	NT	-0.35	-0.01	0.00	6.42	1709.26
QQESPFVMMSAPPAQ	Trypsin, Clostripain IodosoBenzoate, Trypsin_K Trypsin_R,AspN	NA	NT	-0.23	-0.08	-1.00		1648.09

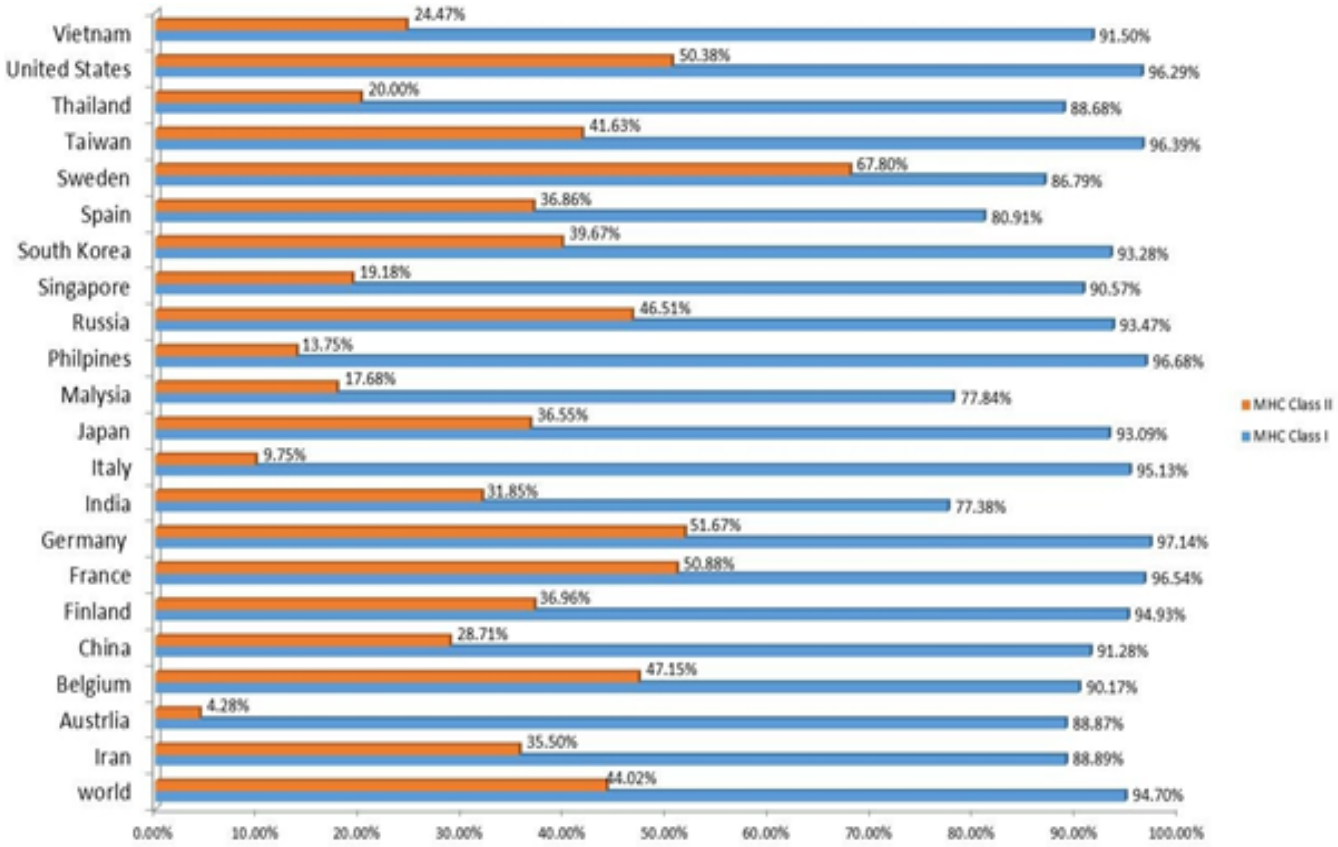

Figure 5: a) Population Coverage of MHC class I and MHC class II around the globe predicted by IEDB population Coverage Tool

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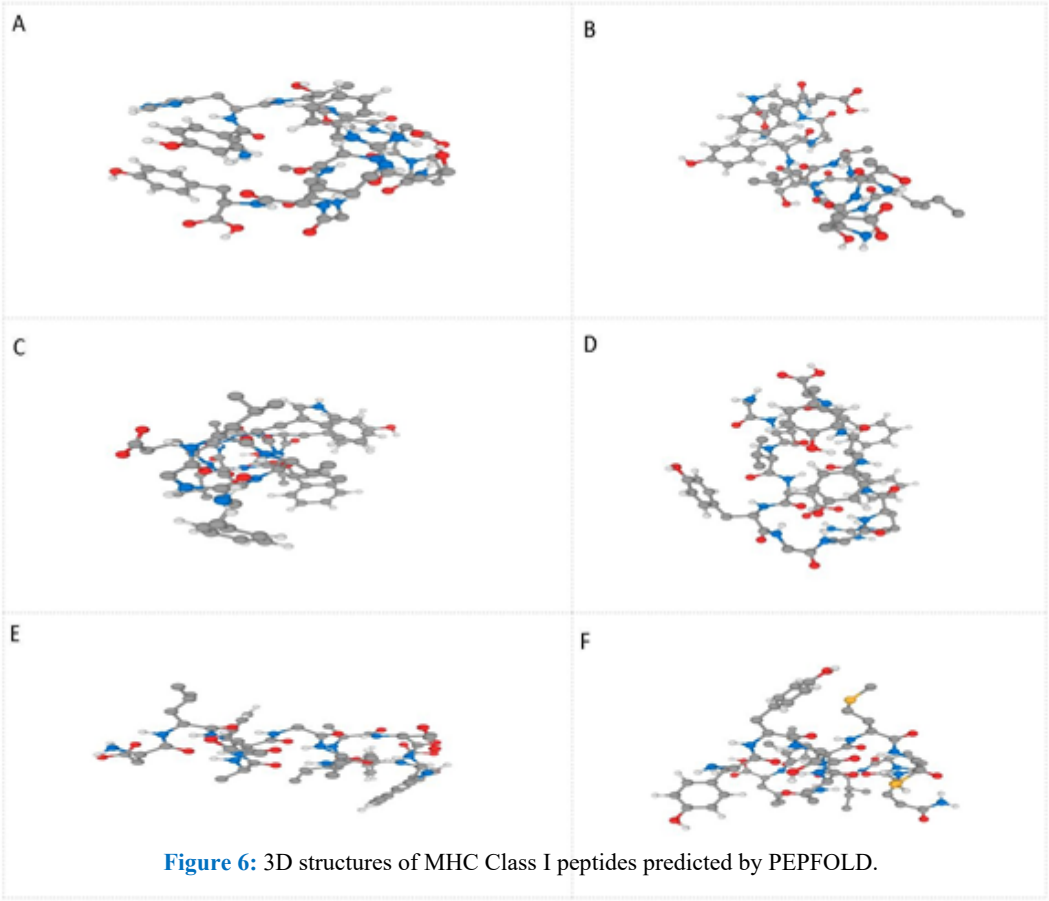

Figure 6: 3D structures of MHC Class I peptides predicted by PEPFOLD.

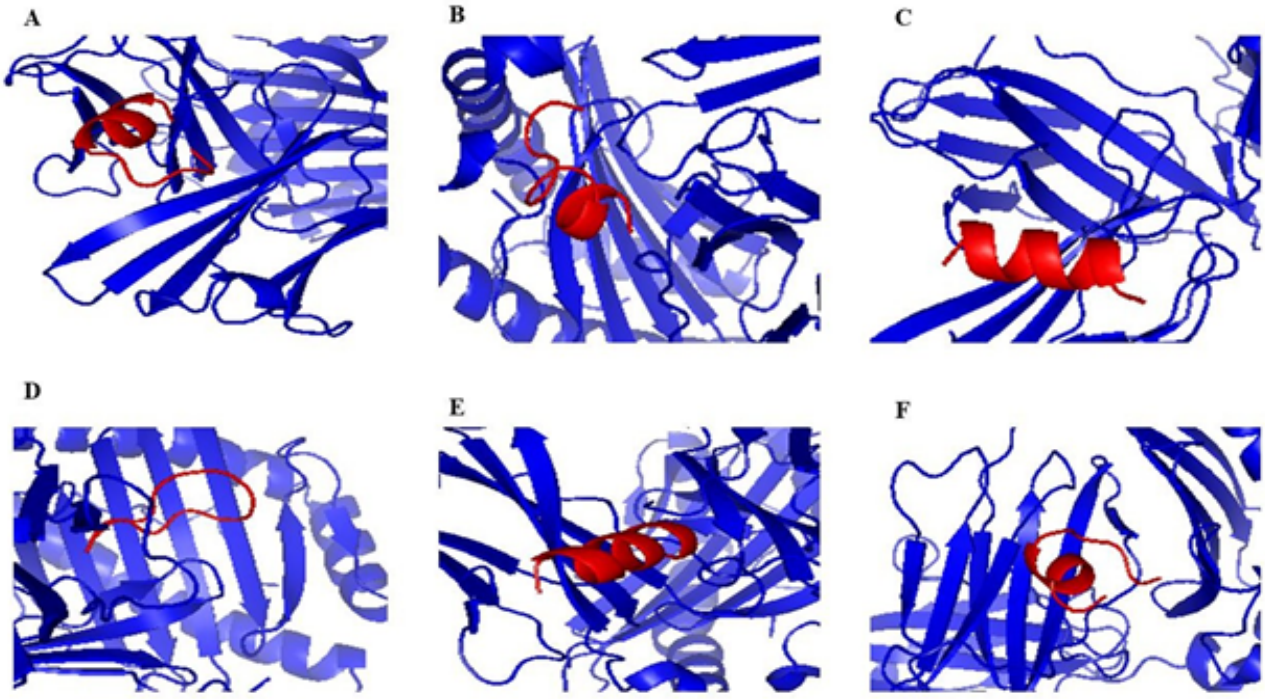

Figure 7: The 3D binding pattern of the selected 6 peptides (red) docked with HLA-B7 allele (blue).

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Discussion

Several viral infections appeared through many fatal new viruses and these viruses are disastrous for humans. Therefore, vaccine designing to tackle viruses is difficult in a short period [48]. One of the most dangerous infectious viruses such as the 2019 novel coronavirus also called SARS-CoV-2 identified (10 February 2020) in patients of severe pneumonia in Wuhan (China)[15]. Several methods could be used for the treatment of coronavirus such as vaccine, peptides, monoclonal antibodies but we designed peptides for SARS-CoV-2. Genome analysis of 2019- nCoV reveals that four catalytic sites are conserved among all kinds of coronaviruses therefore it is suggested to redesign the already present inhibitors of MERS and SARS[8]. Genomic RNA of SARS-CoV is replicated with the help of replicasepolyproteins that are activated with the help of two enzyme proteases such as 3C-like protease (3CLpro) and Papain like protease (PLpro)[49]. SARS-CoVPLpro replicates the polyprotein by the conserved cleavage sites that are conserved among coronaviruses. Furthermore, it is suggested that aspartic acid (ASP1826) and four cysteine residues are essential to perform the activity of PLpro in SARS-CoV[50]. The vaccine could be beneficial and cost-effective in preventing the viral attack but biologically it takes years to be designed in active form. So at presentimmunoinformatics is used to make peptide-based vaccine which is biologically safe and designed in less time than in-vitro vaccine [51].With the advancement in bioinformatics techniques such as next-generation sequencing(NGS) and proteomics enables us to design effective vaccine bases on peptide through the computational immunology (Immunoinformatics)[52, 53].

The development of the peptide based vaccine was explored in this study targeting the papain- like protease protein of the SARS-COV-2. Primary, secondary, and tertiary structure levels of the protein were analyzed. The primary structure of the protein was analyzed by protparam which indicates that protein was 217252.61 kDa in molecular weight. Protein was acidic according to its theoretical PI value. The calculated aliphatic index and instability index values showed the thermostability and stability of the protein. A negative score of the grand average of hydropathy indicates the hydrophilic nature that renders its interaction with neighboring water molecules. Protein was found to be antigenic, immunogenic and non-allergenic indicating the potential to cause robust immune response without any allergic reactions.

B & T cell epitopes of the target protein were forecasted to assist the immune response of the host.Forecasting T cell &B cell is an important step in vaccine development; therefore both types of epitopes were predicted by the protein sequence and their antigenicity was assessed. ABCpred and Discotope 2.0 servers were used to predict linear and discontinuous B cell epitopes respectively. Different IEDB techniques were used to access solvent accessibility, antigenicity, disulphide bonds, and flexibility. B cell epitopes that were antigenic and present on the outer surface were considered. 'KPLEFGATSAALQP' and 'EDDYQGKPLEFGAT' had high antigenicity (1.7) and score among B cells. Furthermore, the IEDB consensus approach predicts antigenic T cell determinants with the ability to bind MHC class I and MHC class II. Antigenic, non-allergenic and conserved T cell epitopes that were bound to multiple alleles were considered. YHTTDPSFLGRY' in MHC class I and 'PFVMMSAPPAQYELK' in MHC class II had the highest antigenicity among T cell epitopes. Pymol visualized the location of peptides on the 3D protein structure. Vaccine's efficacy depends on the population in which the vaccine is being used. MHC class I and MHC class II epitopes that were selected represent 94.70% and 44.02% of the world's population respectively, indicating vaccine developed would be effective for most of the world population. Allergenicity, toxicity and physiochemical properties of predicted epitopes have also been tested for further improvement in specificity and selection. Digestion analysis tests peptideprotection and stability.Epitopes identified during analysis should be tested for the therapeutic potential for futures studies.

Conclusion

A reverse vaccinology approach was implemented in this study to recognize surface-exposed peptides, instead of concentrating on the entire pathogen, an inefficient and effective procedure. B-cells& T-cell epitopes predictedby sequence, conservational, andstructure analysis. B-cell and T- cell epitopes now become vital research due to their predictability, speed, low cost and efficiency. The epitopes with higher antigenicity were selected and these selected peptides would be helpful todesign vaccine against the SARS-COV-2 virus.

Supplementary Files Link

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